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Supporting Information

Dihydrogen Adduct ($Co–H_2$) Complexes Displaying H-Atom and Hydride Transfer

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Supporting Information

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Experimental Details.

1.1 General Considerations.

All manipulations were carried out using standard Schlenk or glovebox techniques. Precursors were prepared under an N_2 atmosphere, but manipulations of H_2 complexes were carried out under an H_2 atmosphere, requiring the rigorous exclusion of N_2 for the anionic complex **[Co](N$_2$)$^\bullet$**. Solvents were deoxygenated and dried by thoroughly sparging with N_2 followed by passage through an activated alumina column in a solvent purification system by SG Water, USA LLC. THF was dried further by stirring over Na/K alloy (>2 h) and were filtered through Celite prior to use. Deuterated benzene was purchased from Cambridge Isotope Laboratories, Inc., and dried by refluxing over Ca-H then distilled and stored over Na. Deuterated THF was purchased from Cambridge Isotope Laboratories and dried over Na/K alloy and was filtered through Celite prior to use. Reagents were purchased from commercial vendors and used without further purification unless otherwise noted. P_3^BCoBr, $P_3^BCo(H_2)$,[1] $[P_3^BCo][BAr^F{}_4]$,[2] and $^tBu_3ArO^\bullet$[3] were prepared according to previously reported protocols. $^tBu_3ArO^\bullet$ as prepared and stored contained ^{t}BuArO-H as a minor component. The fraction of $^tBu_3ArO^\bullet$ was quantified by UV-Visible spectroscopy prior to use.

1.2 Physical Methods.

NMR spectra (^{1}H, ^{31}P, and ^{11}B) were collected at room temperature (25 °C unless specified) on Varian 300, 400, or 500 MHz spectrometers. ^{2}H NMR spectra were collected at room temperature using a Bruker 400 MHz spectrometer. ^{1}H chemical shifts are reported in ppm, relative to tetramethylsilane using residual proton resonances from solvent as internal standards. ^{31}P chemical shifts are reported in ppm relative to 85% aqueous H_3PO_4 and ^{11}B spectra were referenced to $BF_3\bullet Et_2O$. Thin film IR spectra were obtained using a Bruker Alpha Platinum ATR spectrometer with OPUS software in a glovebox under an N_2 atmosphere. UV-Vis measurements were collected using a Cary 50 instrument with Cary WinUV software. Variable temperature experiments were carried out using a UNISOKU cryostat.

X-Ray diffraction and combustion analysis measurements were carried out in the Beckman Institute Crystallography Facility. XRD measurements were collected using a dual source Bruker D8 Kappa diffractometer with a Bruker APEX II. Structures were solved using SHELXT and refined against F^2 on all data by full-matrix least squares with SHELXL. The crystals were mounted on a glass fiber under Paratone N oil. See below for any special refinement details for individual data sets. Combustion analysis measurements were collected using a PerkinElmer 2400 Series II CHN Elemental Analyzer by facility staff.

(1) Suess, D. L. M.; Tsay, C.; Peters, J. C. *J. Am. Chem. Soc.* **2012**, *134*, 14158.
(2) Del Castillo, T. J.; Thompson, N. B.; Suess, D. L. M.; Ung, G.; Peters, J. C. *Inorg. Chem.* **2015**, *54*, 9256-9262.
(3) Manner, V. W.; Markle, T. F.; Freudenthal, J. H.; Roth, J. P.; Mayer, J. M. *Chem. Commun.* **2008**, 256-258.

2. Synthetic Details.

$[P_3^BCo(H_2)][K(THF)_n]$ $[Co](H_2)^{1-}$: Solutions of **$[Co](H_2)^{1-}$** for spectroscopic characterization and reactivity studies were prepared *in situ*. Rigorous exclusion of N_2 from these reactions is necessary to avoid formation of **$[Co](N_2)^{1-}$**. When Na naphthalenide was used as the reductant, it was prepared as a stock solution of known concentration in a septum-capped vial and stored under an Ar atmosphere at -35 ºC. A solution of P_3^BCoBr was prepared in THF and transferred to a Schlenk tube with a Kontes valve seal. This solution was degassed by three freeze-pump-thaw cycles and backfilled with an atmosphere of H_2. Against positive H_2 pressure 2.05 equivalents of Na naphthalenide were added *via* syringe and the mixture was manually stirred at room temperature, rapidly turning dark red. For reductions using Na or K metal, an excess of the solid reductant was added to the Schlenk tube, which was then sealed, rapidly transferred from the glovebox and frozen. The solutions were degassed by three freeze-pump-thaw cycles then backfilled with H_2 and stirred at room temperature overnight. Manipulations of the product including transfers to alternative vessels for characterization and reactivity studies were carried out *via* syringe with high overpressures of H_2. ^{1}H NMR (THF-d_8, 400 MHz): δ 7.38 (3H), 6.90 (3H), 6.61 (3H), 6.45 (3H), 1.98 (6H), 0.84 (18H), 0.34 (18H), -8.60 (br, 2H).^{1}H NMR (THF-d_8, 400 MHz; HD): δ -8.6 (J_{HD} = 29.5 Hz). ^{31}P{^{1}H} NMR (THF, 121 MHz): δ 74.5. ^{11}B{^{1}H} NMR (THF-d_8, 128 MHz): δ 11.1.

$P_3^BCo(H)$/$P_3^BCo(H)(N_2)$ [Co](H)/[Co](H)(N_2): A stirred solution of $[P_3^BCo][BAr^F]$ (150.2 mg) in THF (8 mL) was cooled to -78 °C and a solution of $KHBEt_3$ in THF (1 M, 100 µL, 1 equiv) was added. The reaction mixture was allowed to warm slowly to room temperature overnight, turning dark green. The solvent was removed *in vacuo* and the dark green residue was triturated with pentane (~3 mL) , which was subsequently removed *in vacuo*. The resultant dark green powder was extracted into pentane until washings became nearly colorless (~15 mL total), with removal of the solvent yielding the product in moderate yields (71%) and high purities (~95% as judged by NMR spectroscopy). A minor amount of $P_3^BCo(N_2)$ **$[Co](N_2)^{\bullet}$** was typically observed in materials isolated according to this protocol. Further purification of **[Co](H)/[Co](H)(N_2)** was achieved first by crystallizing the complex (evaporation of an Et_2O solution into MeCy) and then washing the resultant dark green crystals with pentane at -78 °C. The NMR behavior of this species is complicated by N_2/H_2 binding: see below for the detailed spectra for this complex. ^{1}H NMR

(toluene-d_8, 500 MHz, 20 °C; under vacuum): 7.6-7.2 (br, overlapping, 6H), 7.0-6.85 (br, overlapping solvent, 6H), 2.39 (br, 6H), 1.4-0.5 (br, overlapping, 36H). ^{31}P NMR (toluene-d_8, 202 MHz, -40°C, under vacuum): δ 77.05 (d, J = 155 Hz), 63.35, 54.13 (d, J = 155 Hz). IR spectrum (thin film): $\nu_{Co\text{-}H}$ = 1943 cm^{-1}. Anal. Calcd. for $C_{36}H_{55}BCoP_3$: C, 66.47; H, 8.52; N, 0.00. Found: C, 66.50; H, 8.15; N, < 0.1.

3. NMR Spectra.

$[P_3^BCo(H_2)][K(THF)_n]$ ($[Co](H_2)^{1-}$):

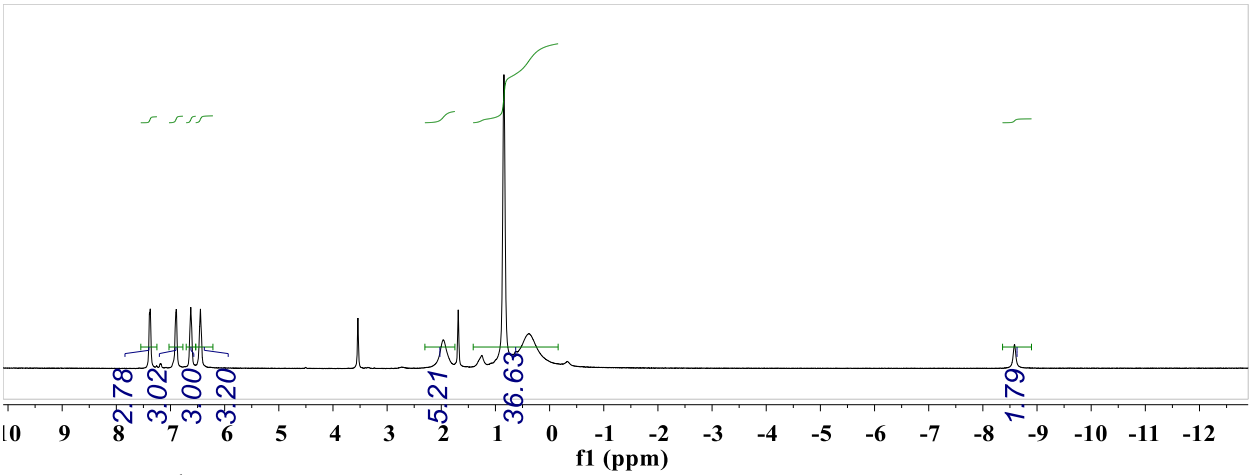


Figure S3.1. ^{1}H NMR spectrum (400 MHz) of **$[Co](H_2)^{1-}$** in THF-d_8.

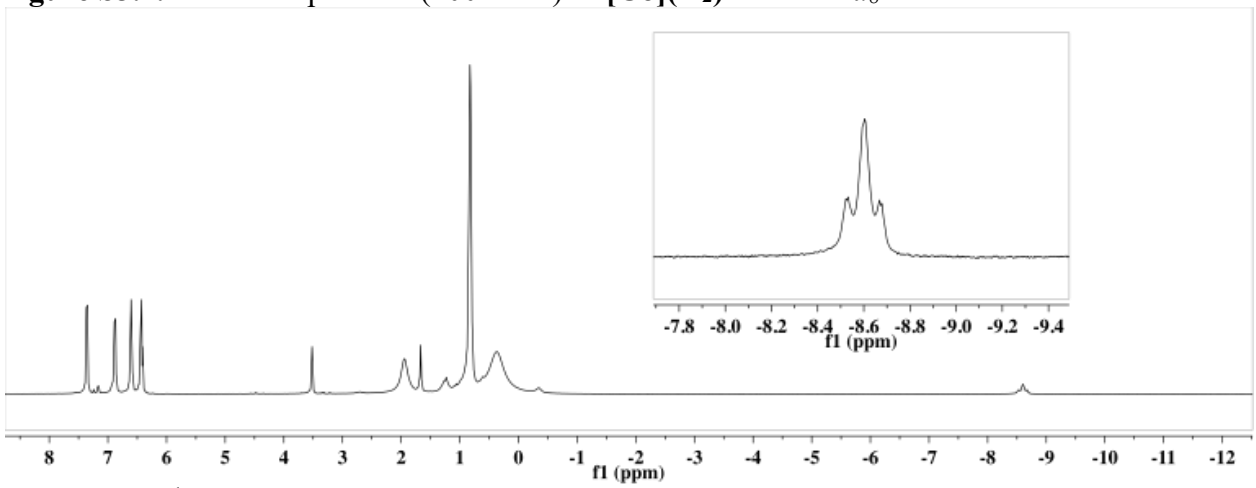


Figure S3.2. ^{1}H NMR spectrum (400 MHz) of **$[Co](HD)^{1-}$** in THF-d_8 with a 1:1 mixture of H_2 and D_2: J_{HD} = 29.5 Hz.

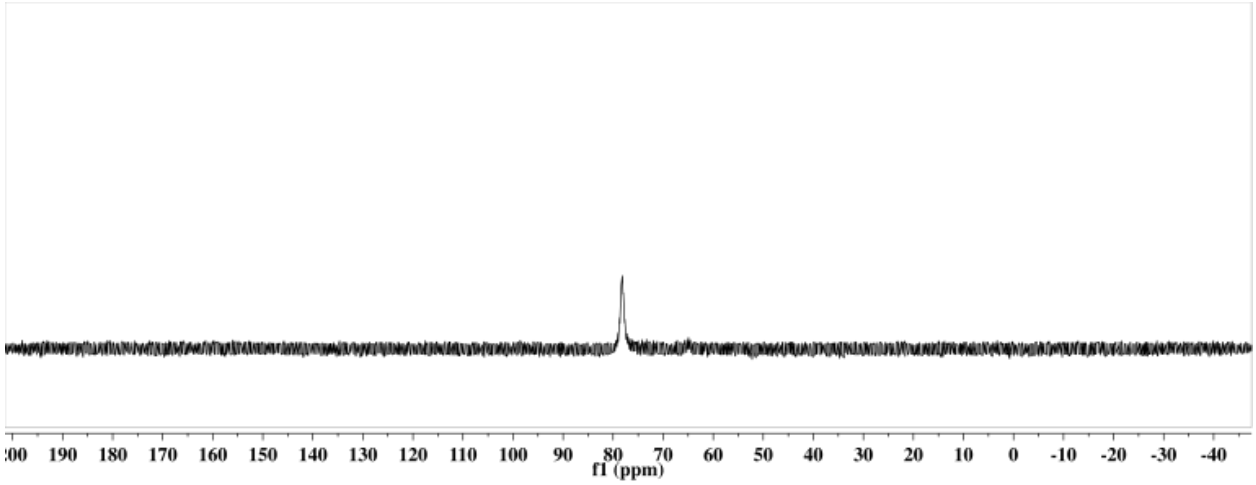


Figure S3.3. ^{31}P NMR spectrum (162 MHz) of **$[Co](H_2)^{1-}$** in THF-d_8.

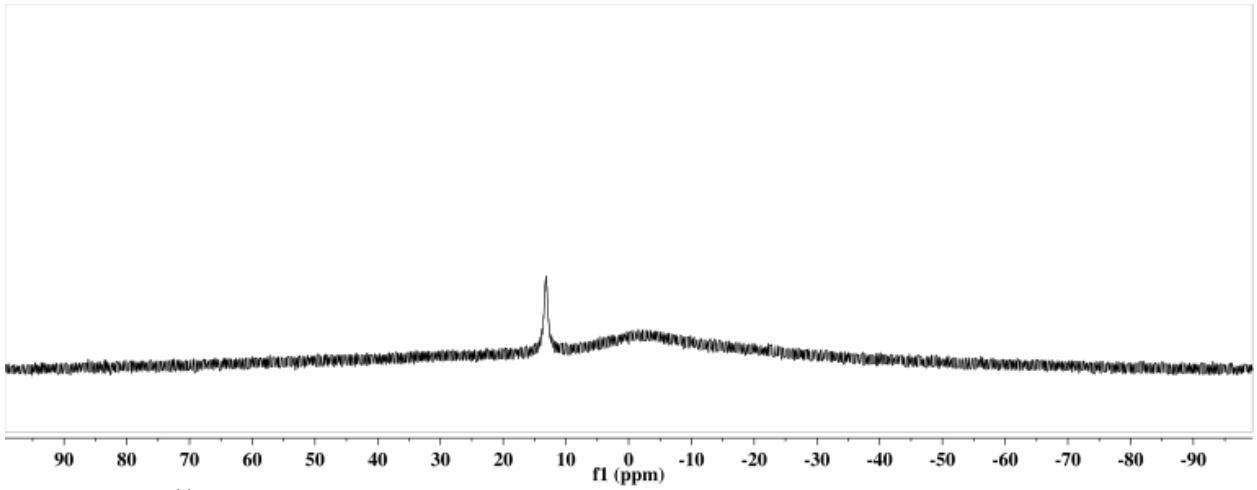


Figure S3.4. ^{11}B NMR spectrum (128 MHz) of **[Co](H$_2$)$^{1-}$** in THF-*d*$_8$.

P$_3^B$Co(H) and N$_2$/H$_2$ binding in solution [Co](H), [Co](H)(N$_2$), and [Co](H)(H$_2$):

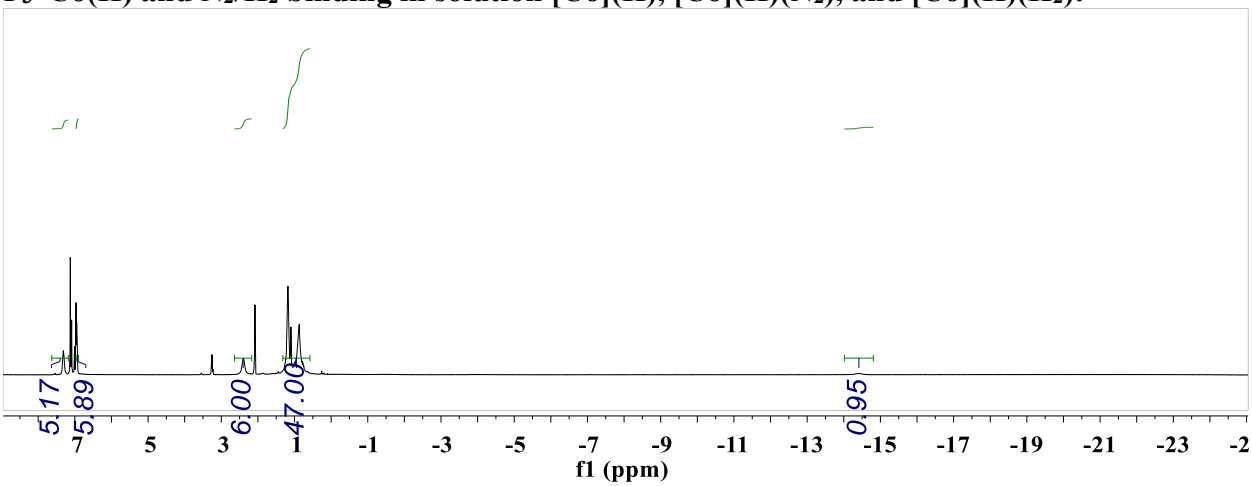


Figure S3.5. ^{1}H NMR spectrum (500 MHz) of **[Co](H)/[Co](H)(N$_2$)** in toluene-*d*$_8$ under an N$_2$ atmosphere.

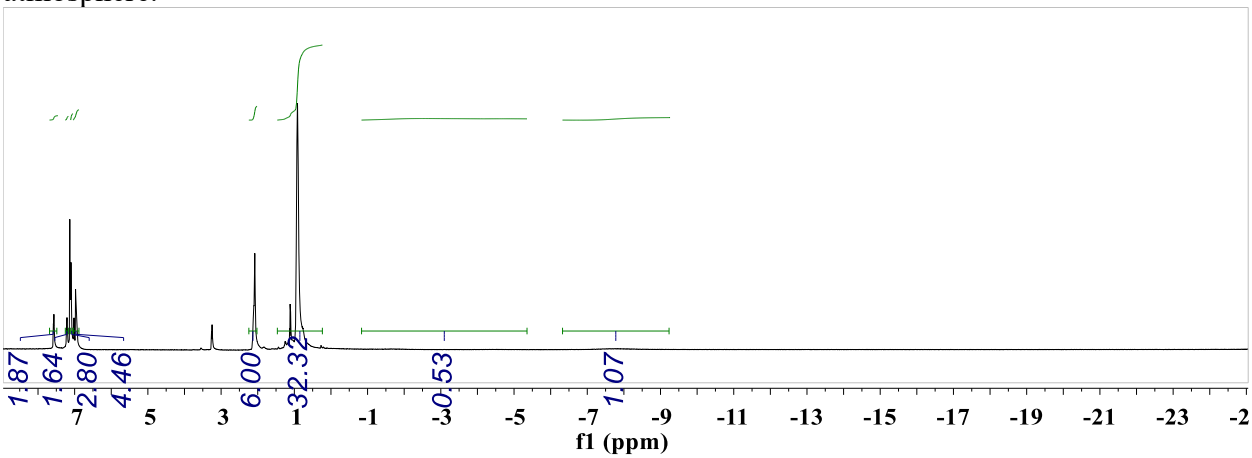


Figure S3.6. ^{1}H NMR spectrum (500 MHz) of **[Co](H)/[Co](H)(H$_2$)** in toluene-*d*$_8$ under an H$_2$ atmosphere at 10 °C.

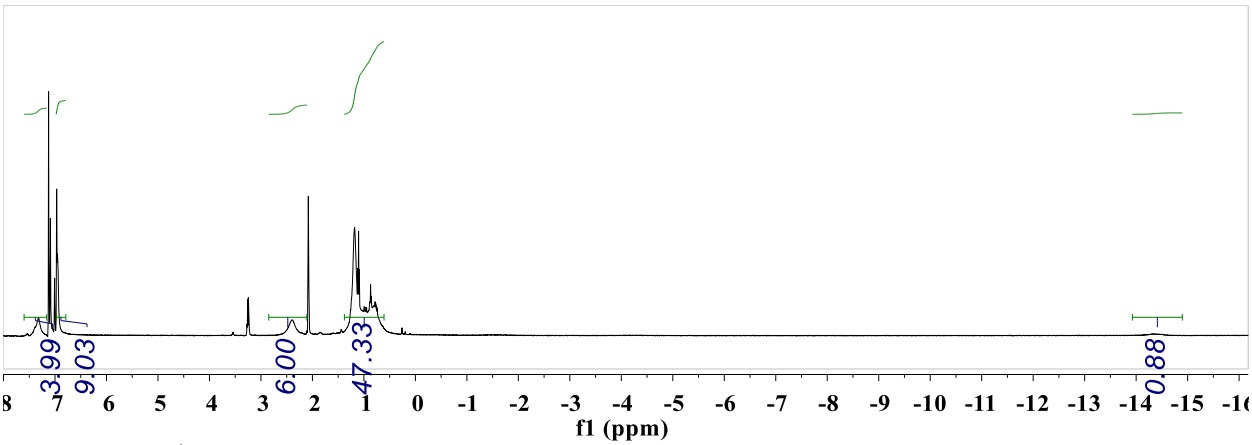


Figure S3.7. ^{1}H NMR spectrum (500 MHz) of **[Co](H)** in toluene-d_8 under vacuum.

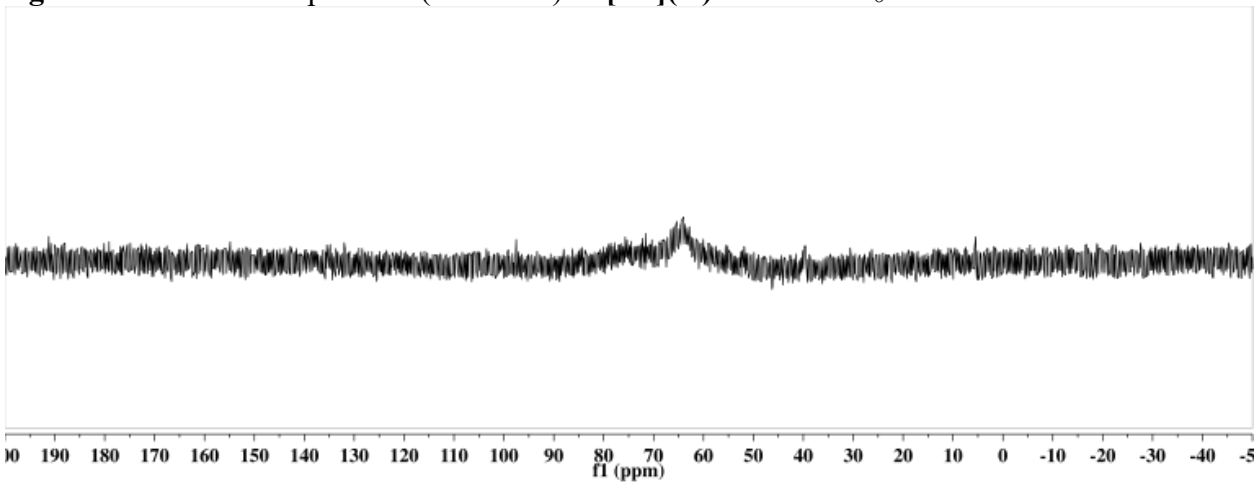


Figure S3.8. ^{31}P NMR spectrum (202 MHz) of **[Co](H)/[Co](H)(N$_2$)** in toluene-d_8 under an N_2 atmosphere at 10 °C.

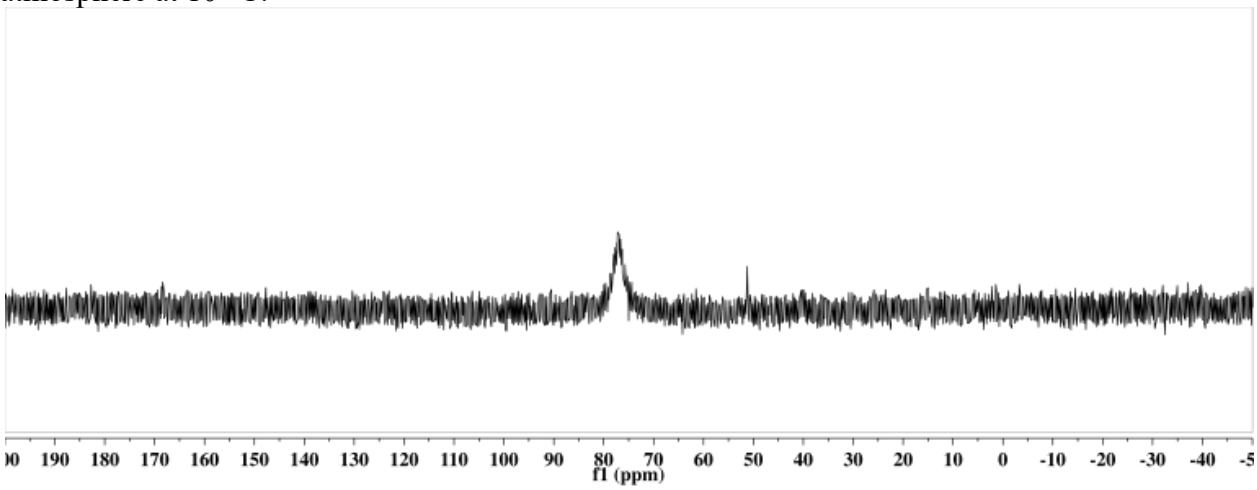


Figure S3.9. ^{31}P NMR spectrum (202 MHz) of **[Co](H)/[Co](H)(H$_2$)** in toluene-d_8 under an H_2 atmosphere.

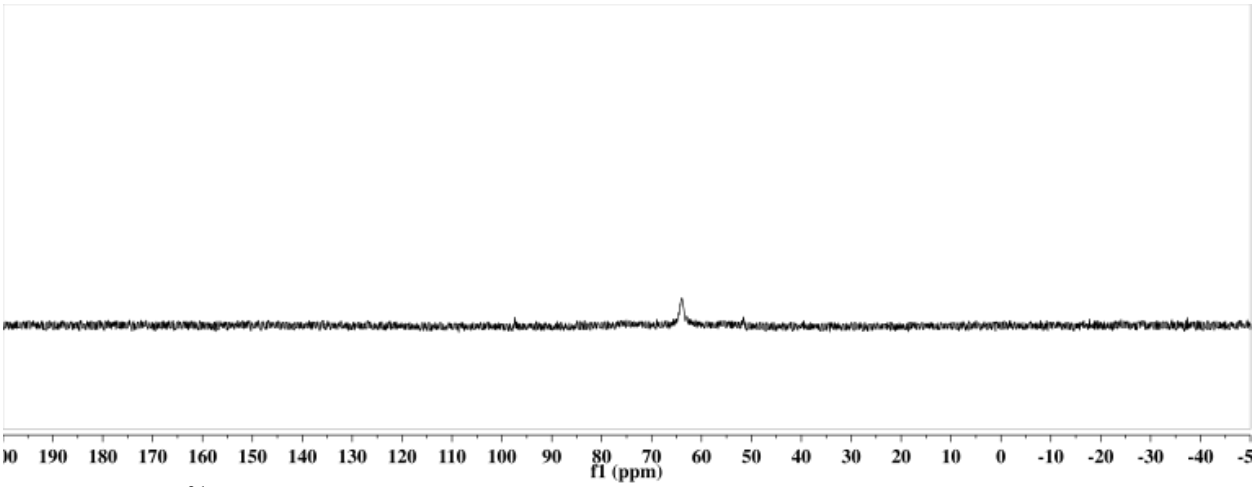


Figure S3.10. ^{31}P NMR spectrum (202 MHz) of **[Co](H)** in toluene-d_8 under vacuum at 20 °C.

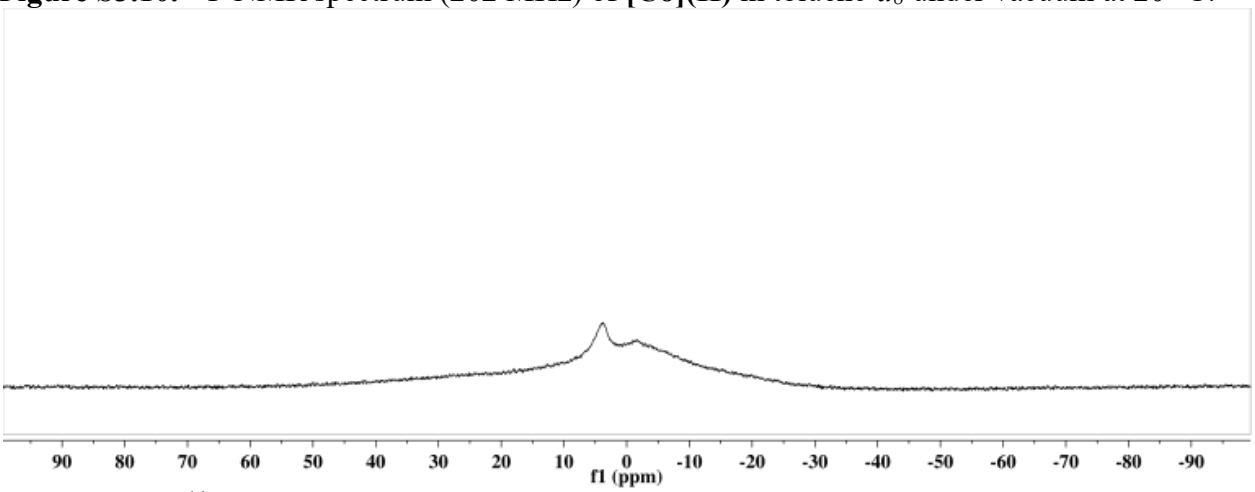


Figure S3.11. ^{11}B NMR spectrum (128 MHz) of **[Co](H)**/**[Co](H)(N$_2$)** in C_6D_6 under an N_2 atmosphere.

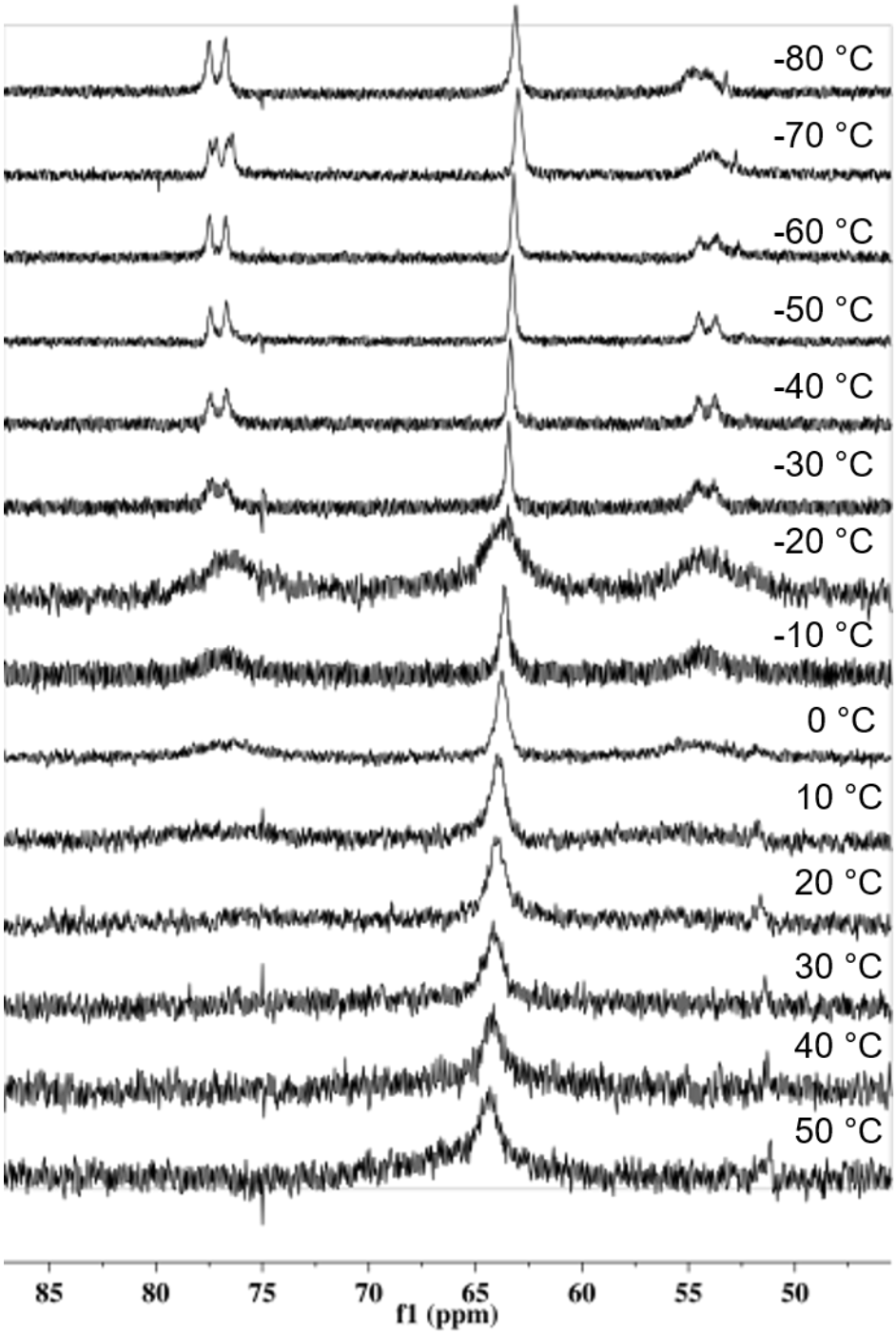


Figure S3.12. Variable temperature ^{31}P NMR spectra (202 MHz) of **[Co](H)** in toluene-d_8 under vacuum from -80 °C (top) to 50 °C (bottom).

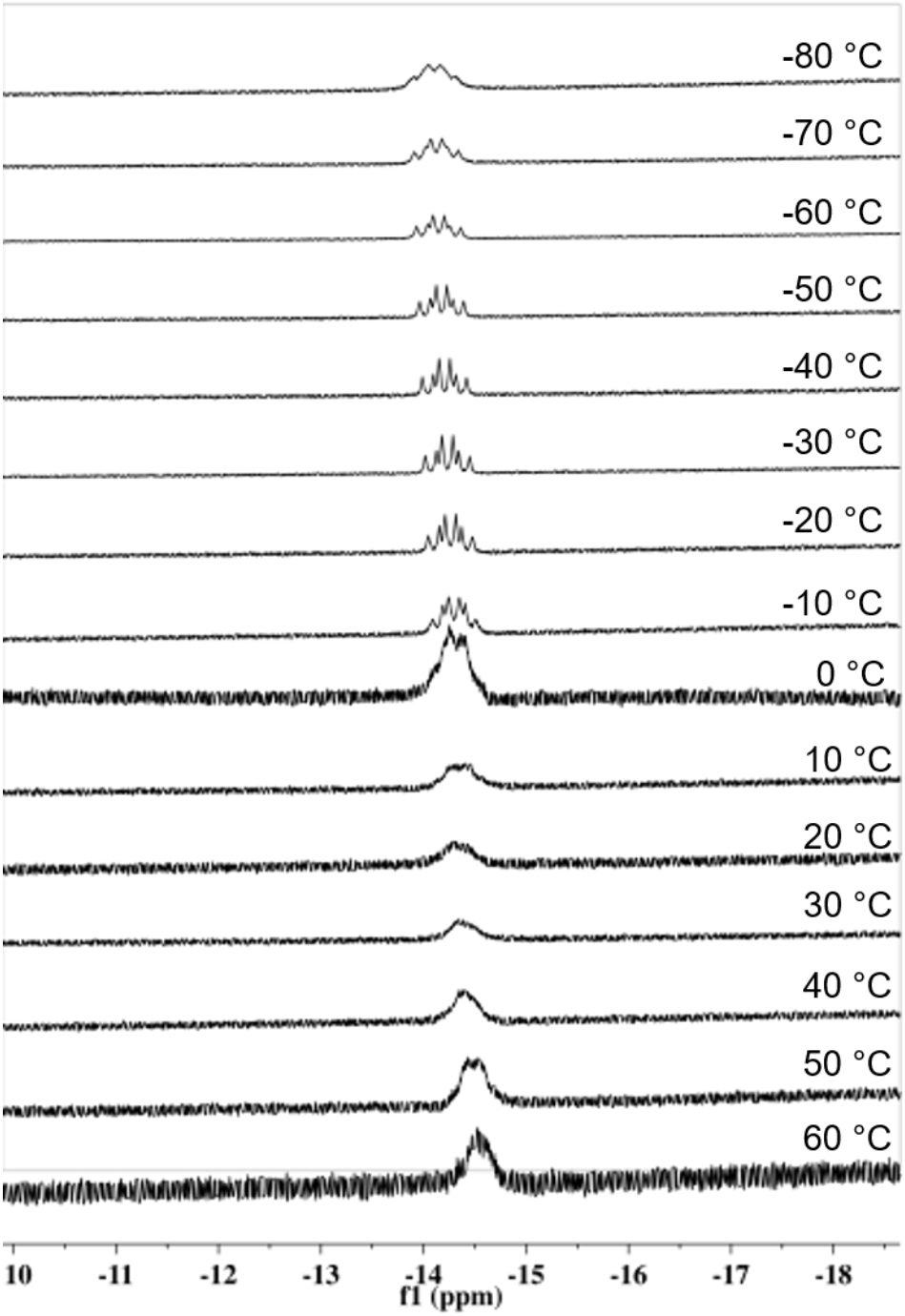


Figure S3.13. Variable temperature ^{1}H NMR (500 MHz) spectra highlighting the hydridic resonance of **[Co](H)** in toluene-d_8 under vacuum from -80 °C (top) to 60 °C (bottom).

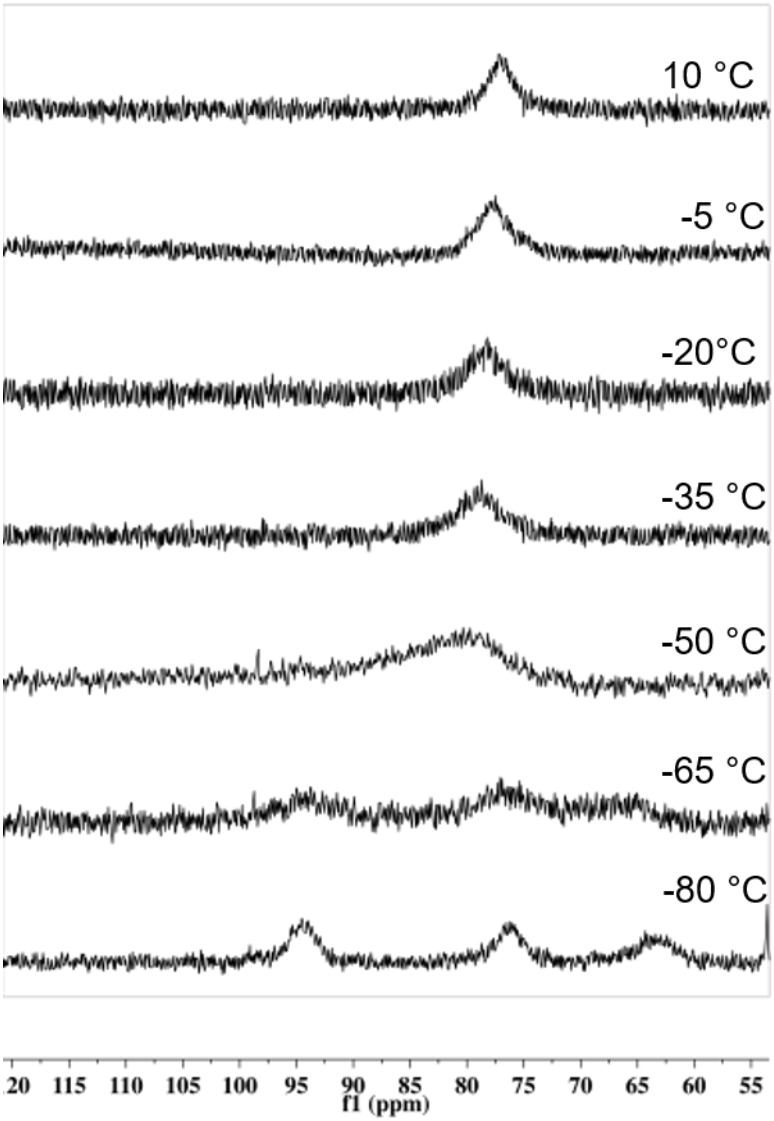


Figure S3.14. Variable temperature ^{31}P NMR (202 MHz) spectra highlighting the hydridic resonance(s) of **[Co](H)/[Co](H)(H$_2$)** in toluene-d_8 under an H_2 atmosphere from 10 °C (top) to -80 °C (bottom).

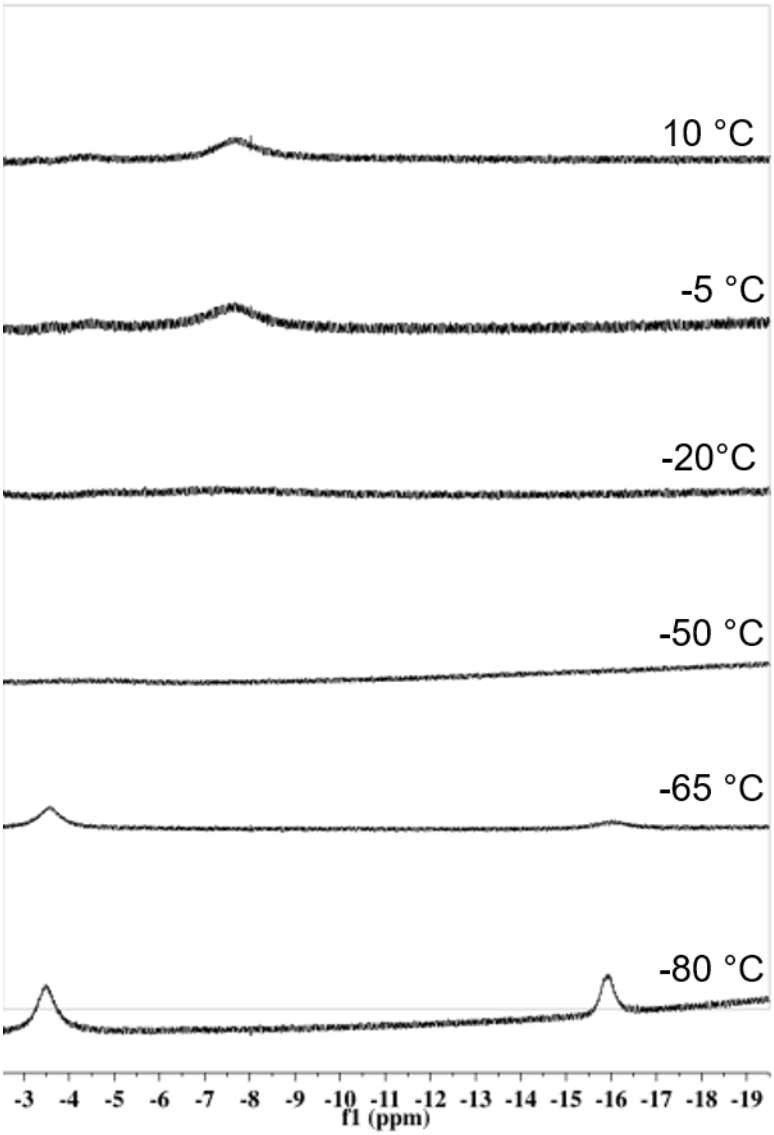


Figure S3.15. Variable temperature ^{1}H NMR (500 MHz) spectra highlighting the hydridic resonance(s) of **[Co](H)/[Co](H)(H$_2$)** in toluene-d_8 under an H_2 atmosphere from -80 °C (bottom) to 10 °C (top).

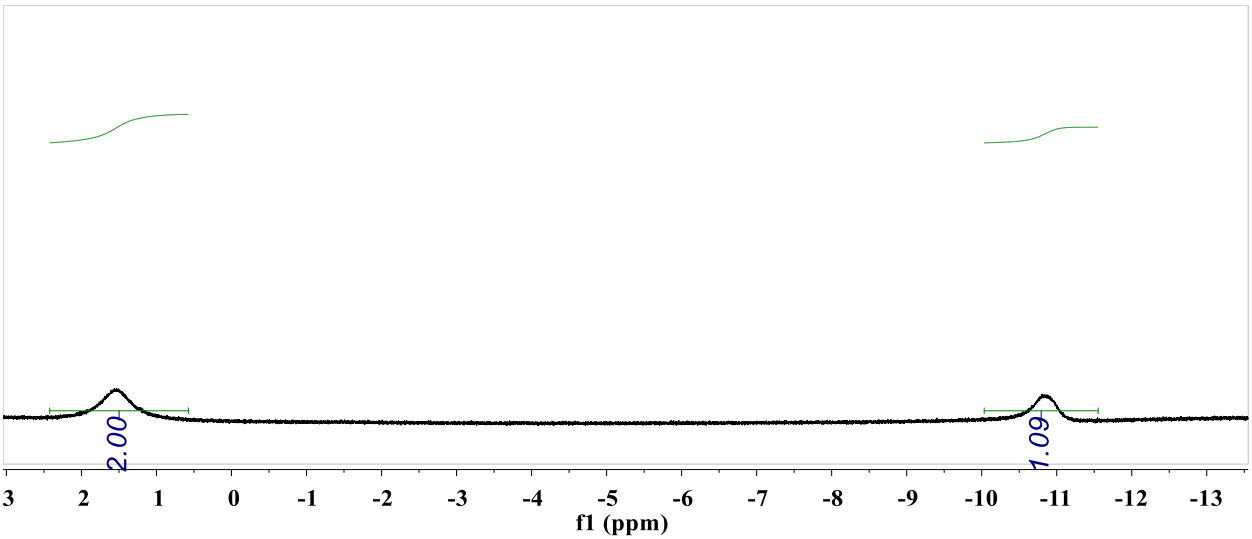


Figure S3.16. ^{1}H NMR (500 MHz) spectrum showing the relative integrations of the hydridic resonance(s) of **[Co](H)/[Co](H)(H$_2$)** at -80 °C.

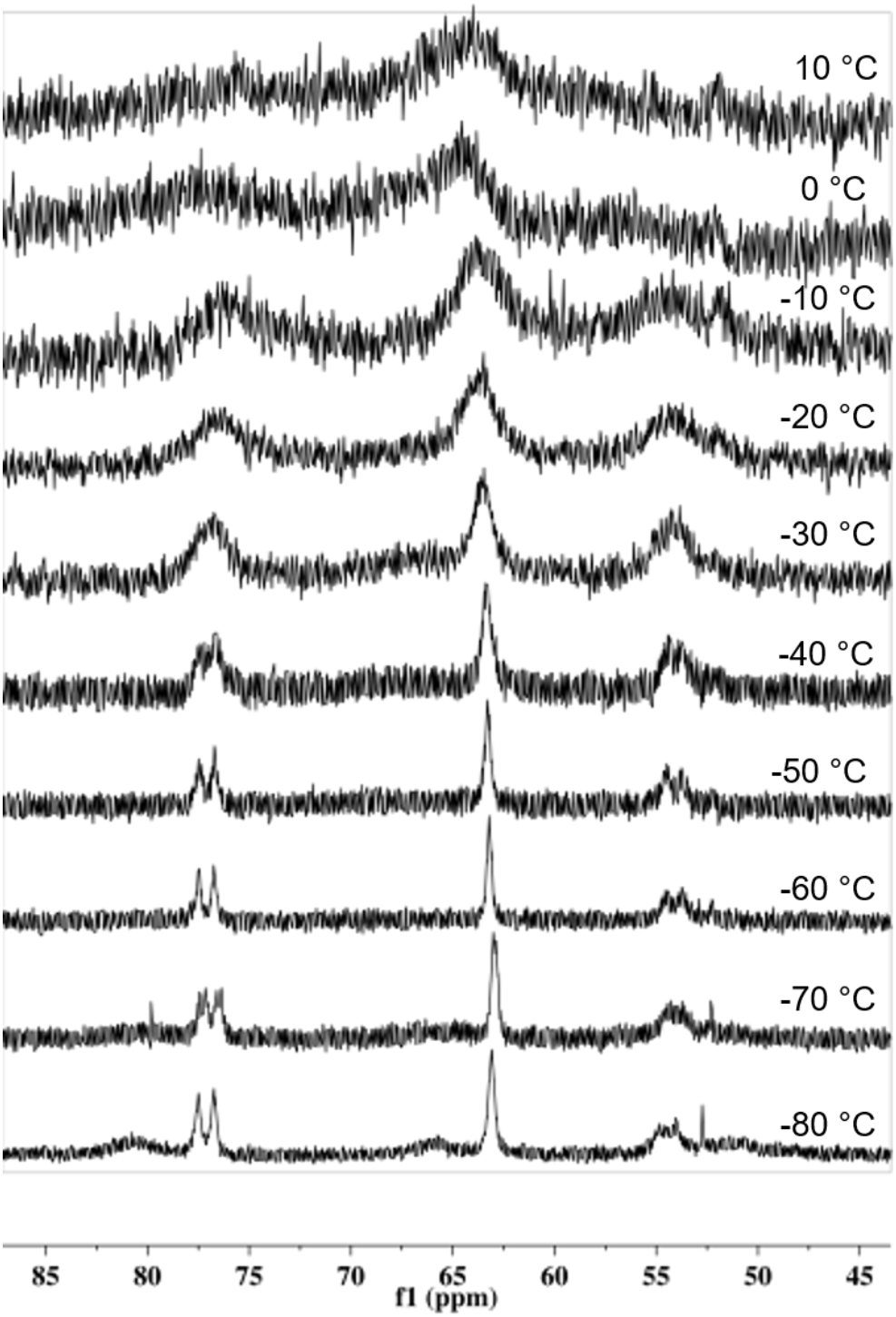


Figure S3.17. Variable temperature ^{31}P NMR spectra (202 MHz) of **[Co](H)/[Co](H)(N_2)** in toluene-d_8 under an N_2 atmosphere from 10 °C (top) to -80 °C (bottom).

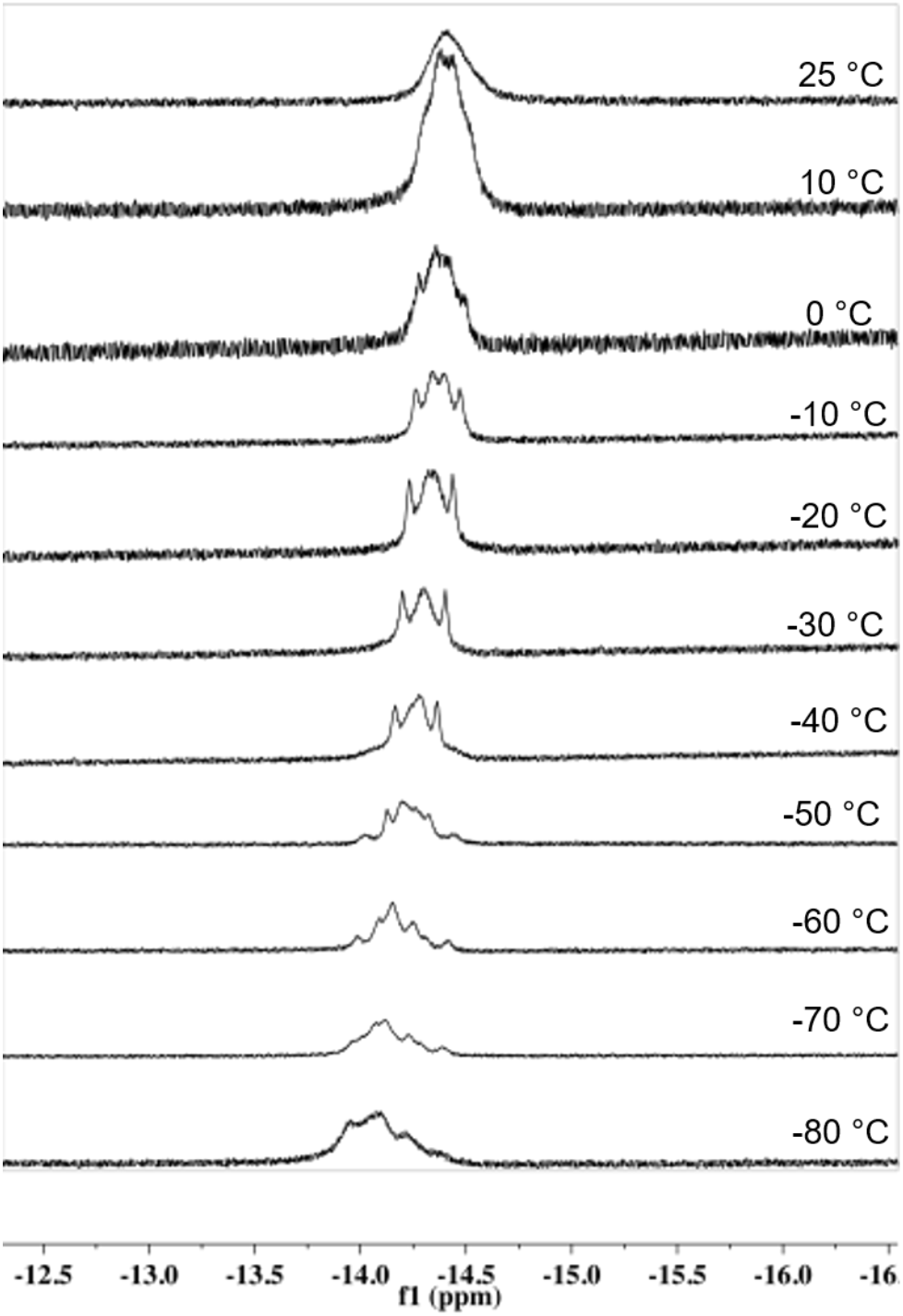


Figure S3.18. Variable temperature ^{1}H NMR (500 MHz) spectra highlighting the hydridic resonance of **[Co](H)**/**[Co](H)(N$_2$)** in toluene-d_8 under an N_2 atmosphere from -80 °C (bottom) to 25 °C (top).

4. Reactivity Studies

Reactivity of [Co](H$_2$)$^\bullet$ with ^{t}Bu$_3$ArO$^\bullet$:

A solution of $P_3^BCo(N_2)$ (12.4 mg, .0183 mmol) and trimethoxybenzene (internal standard; 4.6 mg, .0273 mmol) was prepared in Et_2O (2 mL) in a small Schlenk tube. The solution was degassed (3 x FPT) and backfilled with H_2 to generate $P_3^BCo(H_2)$ **[Co](H$_2$)$^\bullet$**. A solution of ^{t}Bu$_3$ArO$^\bullet$ (1 equiv) in Et_2O was added *via* syringe to the Schlenk tube against positive H_2 pressure and the reaction was mixed, rapidly turning dark green. The solvent was removed *in vacuo* and the residue was redissolved in C_6D_6 for product quantification (85% yield **[Co](H)**). A minor amount of the starting material is also observable in the spectrum.

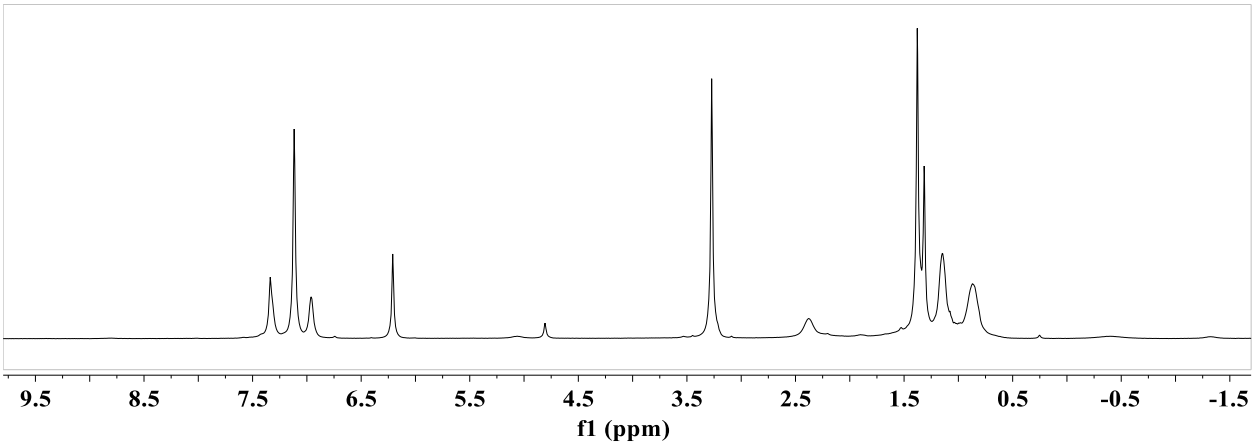


Figure S4.1. Narrow view of the product mixture observed by ^{1}H NMR from the reaction between $P_3^BCo(H_2)$ **[Co](H$_2$)$^\bullet$** and ^{t}Bu$_3$ArO$^\bullet$.

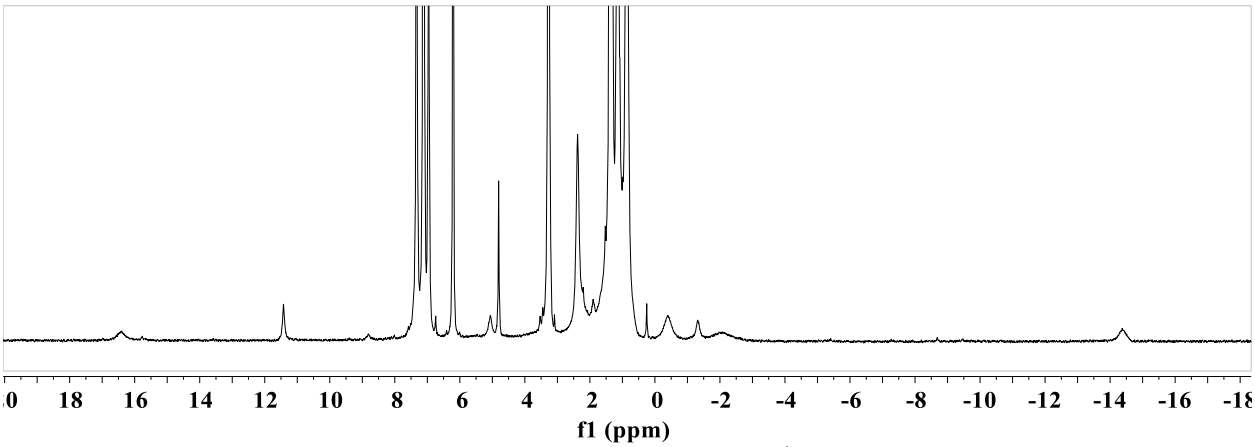


Figure S4.2. Wide view of the product mixture observed by ^{1}H NMR from the reaction between $P_3^BCo(H_2)$ **[Co](H$_2$)$^\bullet$** and ^{t}Bu$_3$ArO$^\bullet$.

Reactivity of [Co](H$_2$)$^{\bullet}$ with TEMPO$^{\bullet}$:

A solution of $P_3^BCo(N_2)$ (12.3 mg, .0182 mmol) and trimethoxybenzene (internal standard; 3.7 mg, .0219 mmol) was prepared in C_6D_6 (0.3 mL) in a J. Young NMR tube. The solution was degassed (3 x FPT) and backfilled with H_2 to generate $P_3^BCo(H_2)$ **[Co](H$_2$)$^{\bullet}$**. A solution of TEMPO$^{\bullet}$ (1 equiv) in C_6D_6 was added *via* syringe to the NMR tube against positive H_2 pressure and the reaction was mixed, slowly turning green over the course of a week. Over this time the starting material is largely consumed, with the concurrent formation of a new, unidentified paramagnetic species as the major product and a minor amount of the Co-H complex **[Co](H)(H$_2$)** (11% yield vs. a trimethoxybenzene internal standard).

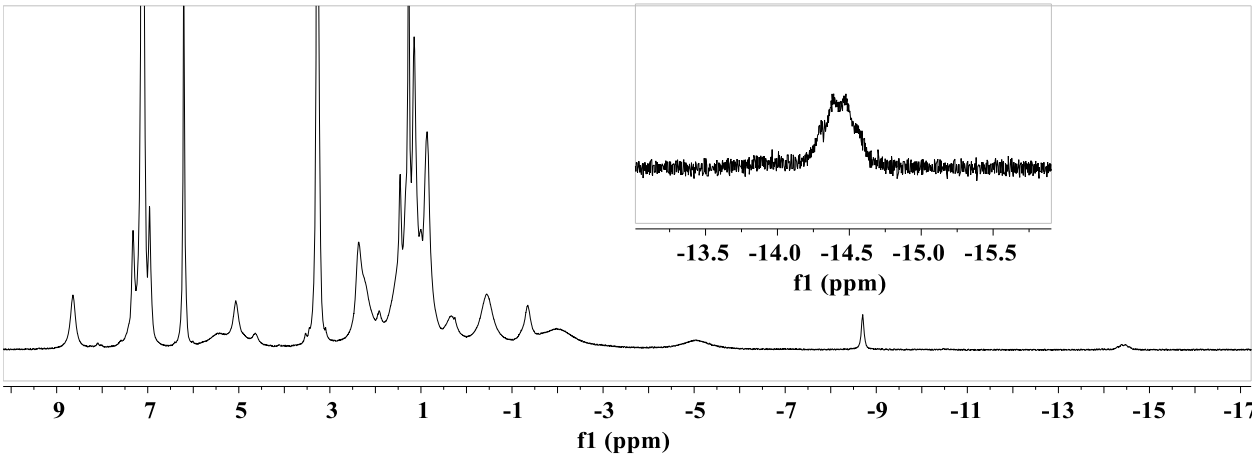


Figure S4.3. Narrow view of the product mixture observed by ^{1}H NMR from the reaction between $P_3^BCo(H_2)$ **[Co](H$_2$)$^{\bullet}$** and TEMPO$^{\bullet}$.

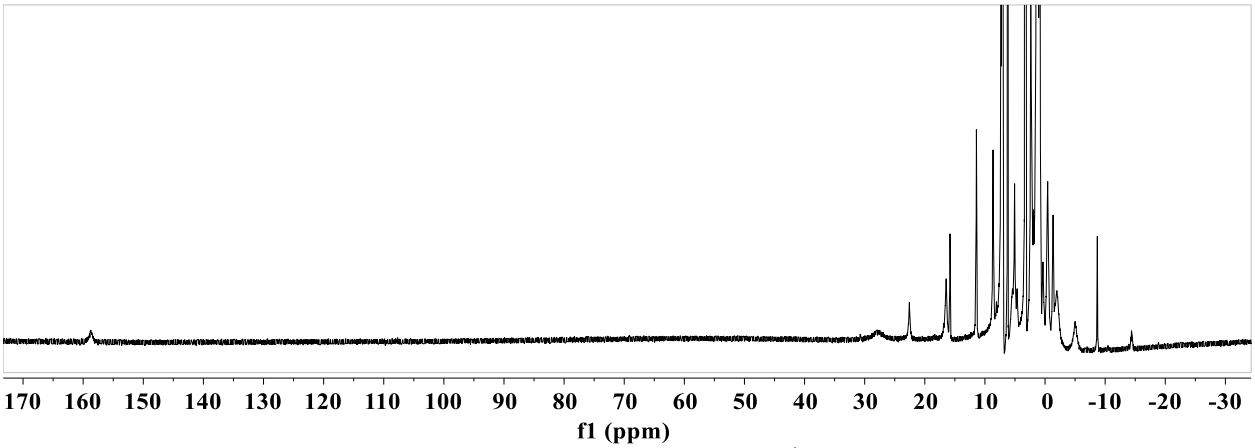


Figure S4.4. Wide view of the product mixture observed by ^{1}H NMR from the reaction between $P_3^BCo(H_2)$ **[Co](H$_2$)$^{\bullet}$** and TEMPO$^{\bullet}$.

Reaction of $[Co](H_2)^{1-}$ with BEt_3:

A solution of $[P_3^BCo(H_2)][Na(solv)_x]$ **$[Co](H_2)^{1-}$** (12.5 mg, 0.0171 mmol) was prepared in THF according to the protocol outlined above using Na naphthalenide (2.5 equiv) as the reductant in a small Schlenk tube in the presence of a trimethoxybenzene internal standard (7.4 mg, .0440 mmol). The solution was stirred and a stock solution of BEt_3 (0.1 M, 330 μL, 1.6 equiv) was added against a positive H_2 overpressure and the reaction was mixed at room temperature for 20 h. The solvent was removed *in vacuo*, and the residue was redissolved in C_6D_6 and the yield of **[Co](H)** was quantified by ^{1}H NMR spectroscopy (86%).

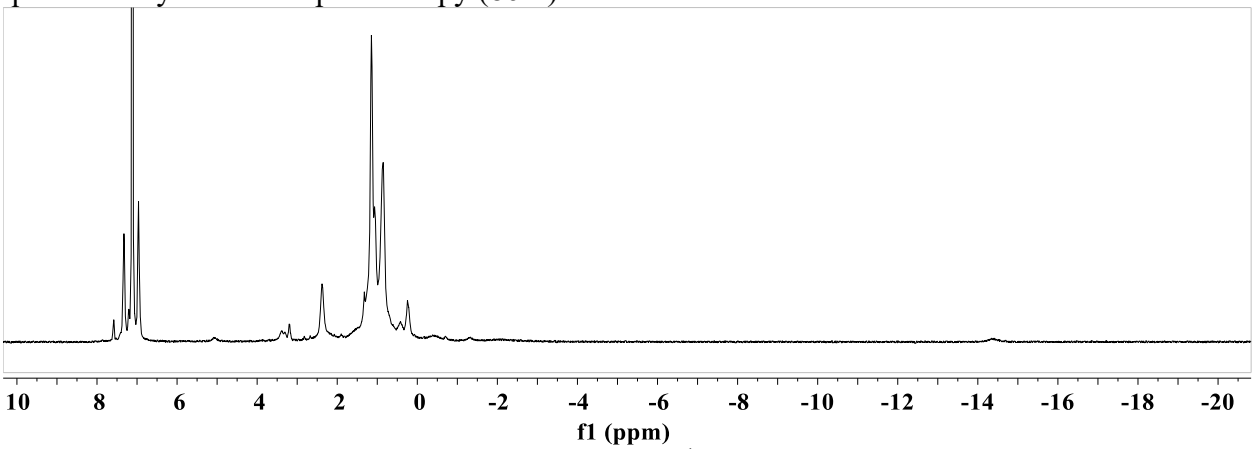


Figure S4.5. Product mixture observed by ^{1}H NMR from the reaction between $[P_3^BCo(H_2)][Na(solv)_x]$ **$[Co](H_2)^{1-}$** and BEt_3.

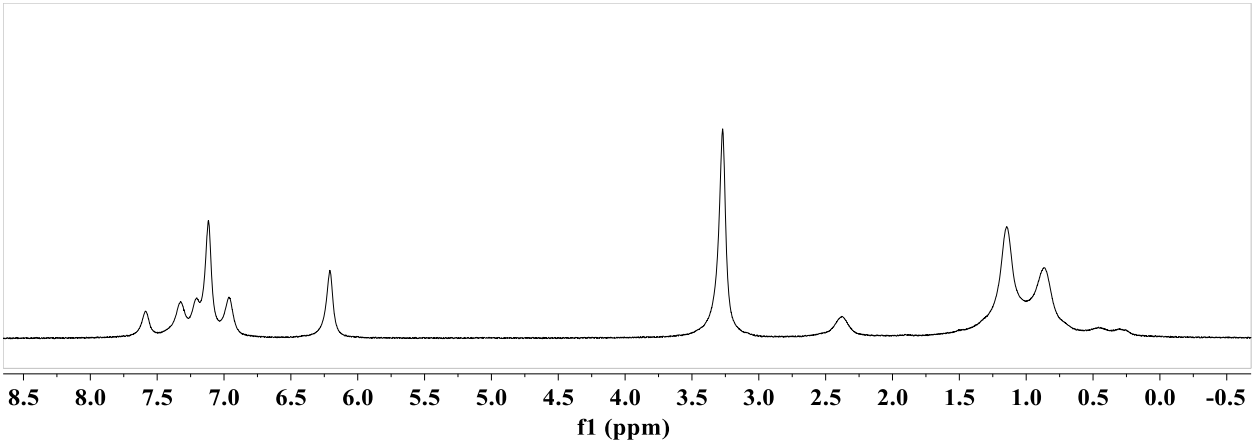


Figure S4.6. Product mixture observed by ^{1}H NMR from the reaction between $[P_3^BCo(H_2)][Na(solv)_x]$ **$[Co](H_2)^{1-}$** and BEt_3 with a trimethoxy benzene internal standard.

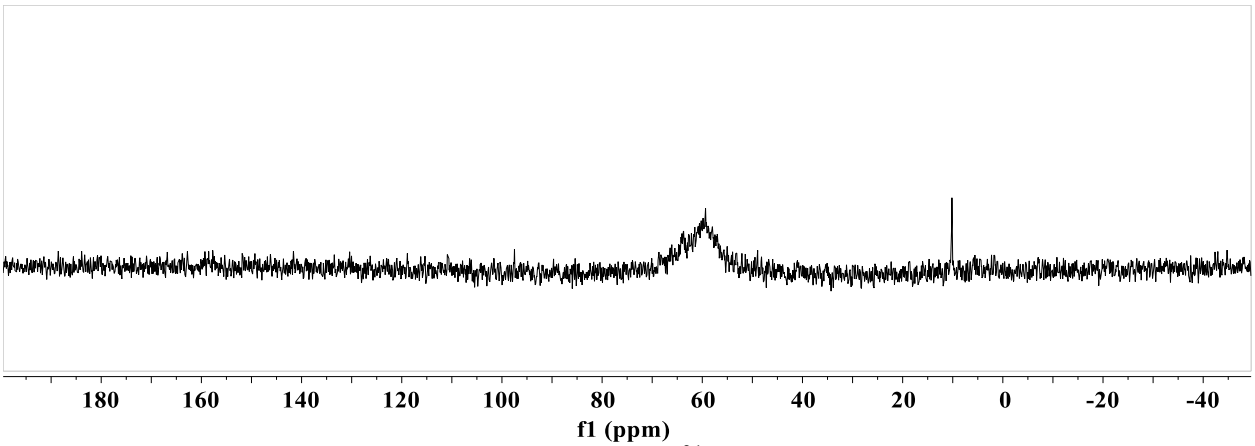


Figure S4.7. Product mixture observed by ^{31}P NMR from the reaction between $[P_3^BCo(H_2)][Na(solv)_x]$ **[Co](H₂)$^{1-}$** and BEt_3.

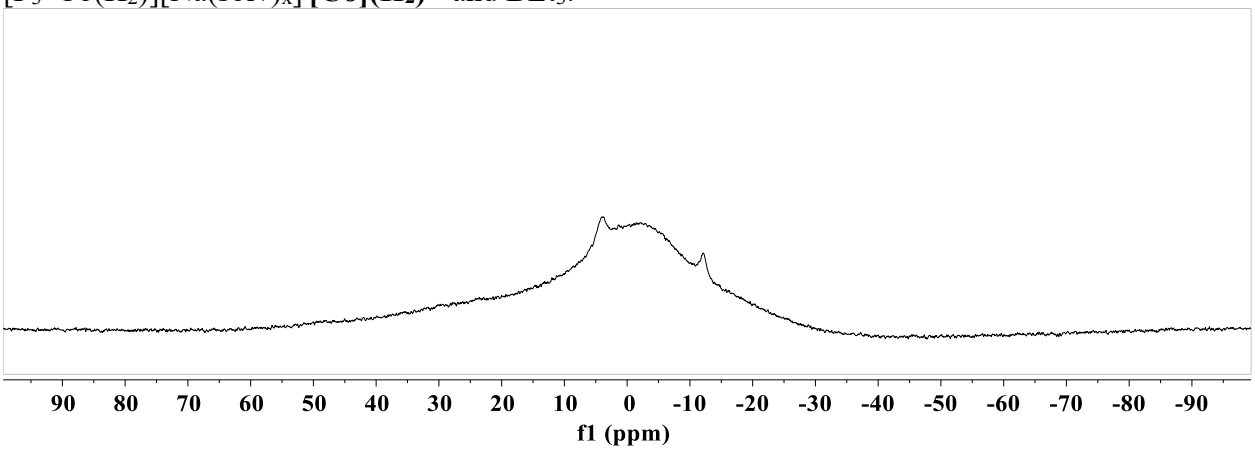


Figure S4.8. Product mixture observed by ^{11}B NMR from the reaction between $[P_3^BCo(H_2)][Na(solv)_x]$ **[Co](H₂)$^{1-}$** and BEt_3.

Reactions Using Deuterium Gas:

For these reactions, we note that H_2/D_2 scrambling into the hydride position for **[Co](H)(H₂)** is observed. This suggests that, regardless of the origin of the H-atom equivalent for the generation of **[Co](H)/[Co](H)(H₂)**, under a D_2 atmosphere, deuterium washes into the Co-H.

H-atom transfer: For this reaction, **[Co](N₂)•** and $^tBu_3ArO^\bullet$ were mixed in benzene (C_6H_6) and the resultant green solution was degassed and D_2 was added, resulting in a rapid paling of the reaction solution. The resultant mixture was separated into two vials and the solvent was removed. One of the vials was analyzed by ^1H NMR and the second by ^2H NMR.

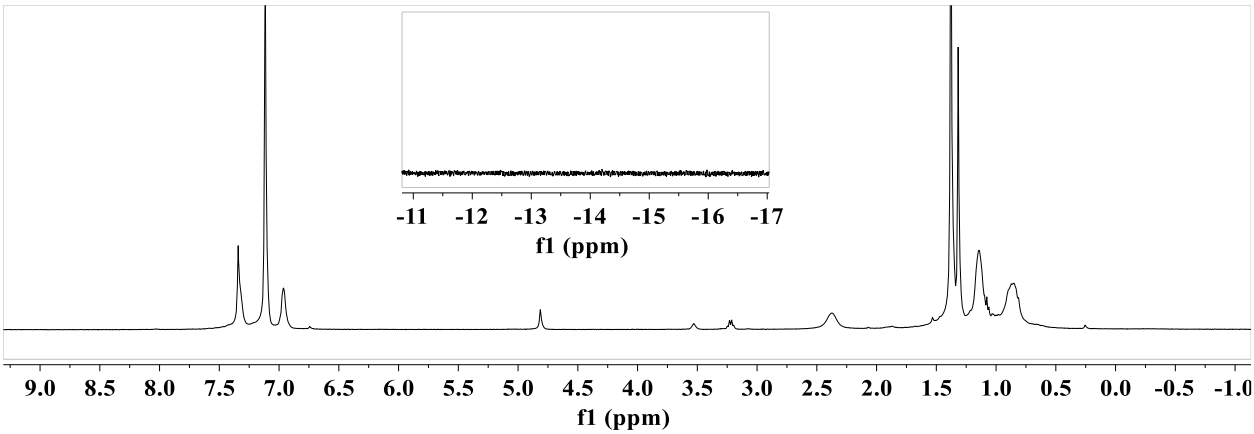


Figure S4.9. ^{1}H NMR spectrum (400 MHz, C_6D_6) of the reaction mixture generated from **[Co](D$_2$)$^{\bullet}$** and ^{t}Bu$_3$ArO$^{\bullet}$. The presence of the O-H peak is, in part, attributable to the presence of a phenol impurity in the starting material.

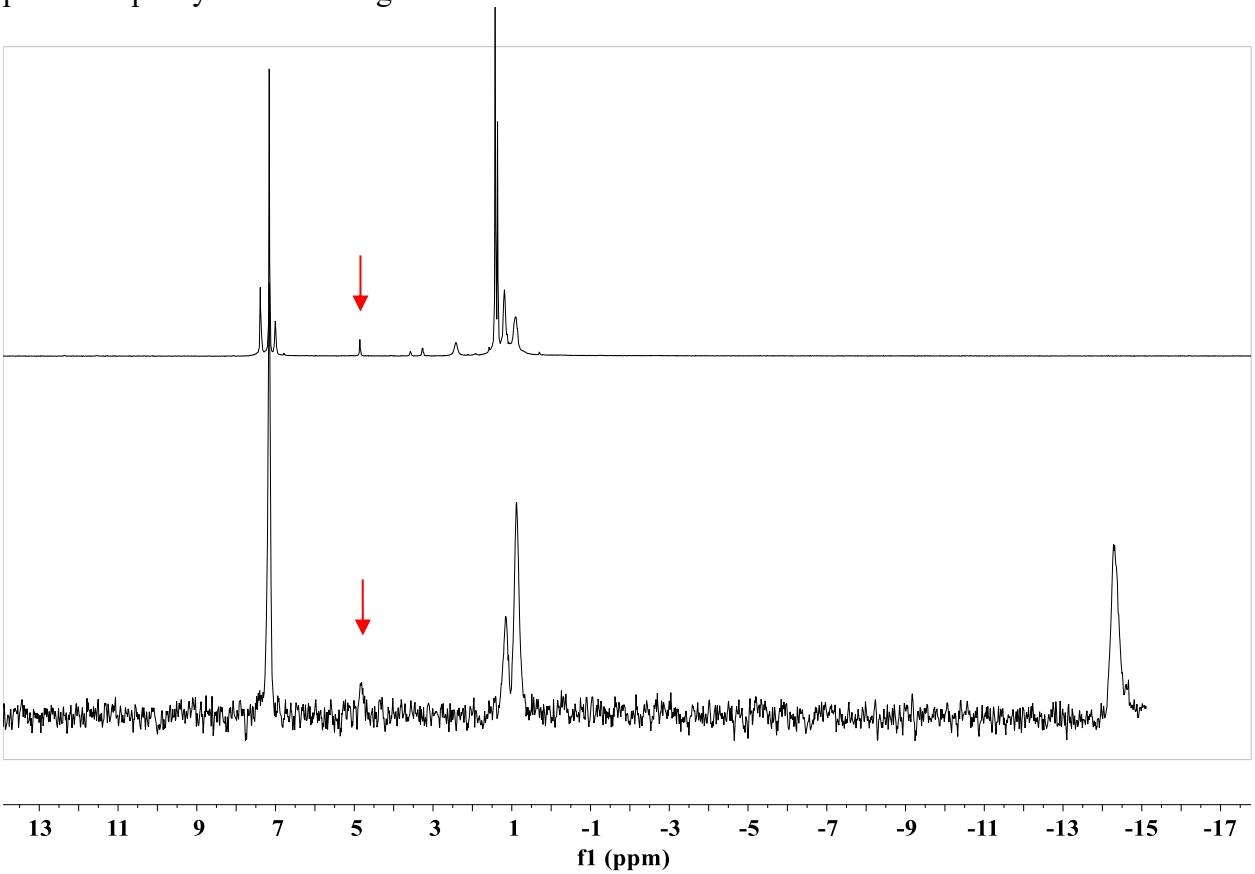


Figure S4.10. Stacked ^{1}H/^{2}H NMR spectra of the reaction mixture generated from **[Co](D$_2$)$^{\bullet}$** and ^{t}Bu$_3$ArO$^{\bullet}$. Scrambling of deuterium into the supporting ligand is apparent in the alkyl region of the spectrum. The presence of both ArO-H and ArO-D is apparent; partial H-atom incorporation may be attributable to the presence of ArO-H in the starting material or derived from scrambling into the ligand.

Hydride transfer: The reactions were set up as above under an H_2 atmosphere. After BEt_3 was added to the reaction mixture, the solution was frozen and the head space was removed and backfilled with D_2. The reaction was thawed and mixed at room temperature for 20 h.

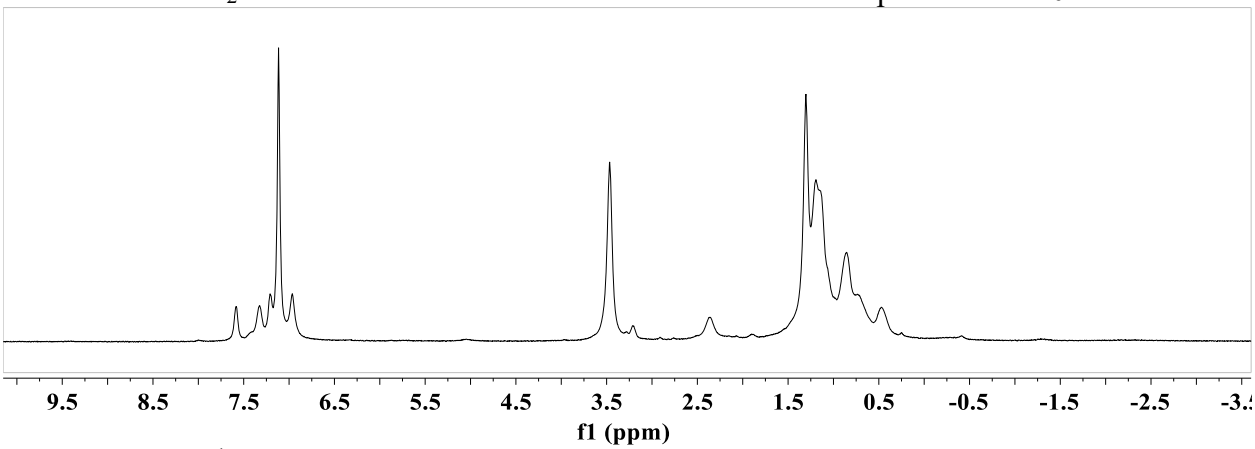


Figure S4.11. ^1H NMR spectrum (400 MHz, C_6D_6) of the reaction mixture generated from **[Co](D₂)**$^{1-}$ and BEt_3.

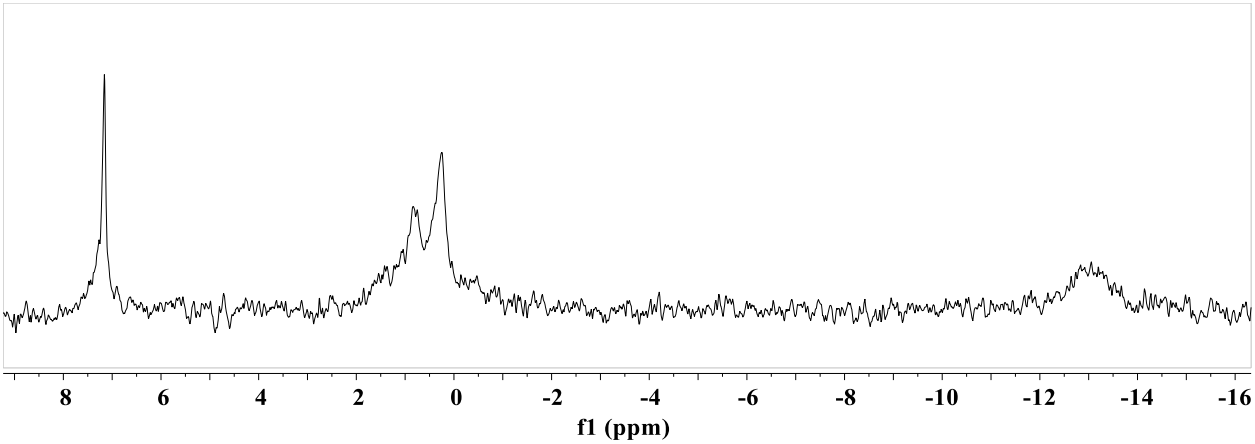


Figure S4.12. ^2H NMR spectrum (MHz, C_6D_6) of the reaction mixture generated from **[Co](D₂)**$^{1-}$ and BEt_3. Scrambling into the ligand is again observed for the hydride complex **[Co](D)/[Co(D)(N₂)**. The position of the borodeuteride is not obvious, as is typical of reported $MHBEt_3$ and confirmed by collection of an authentic ^1H spectrum of $KHBEt_3$.

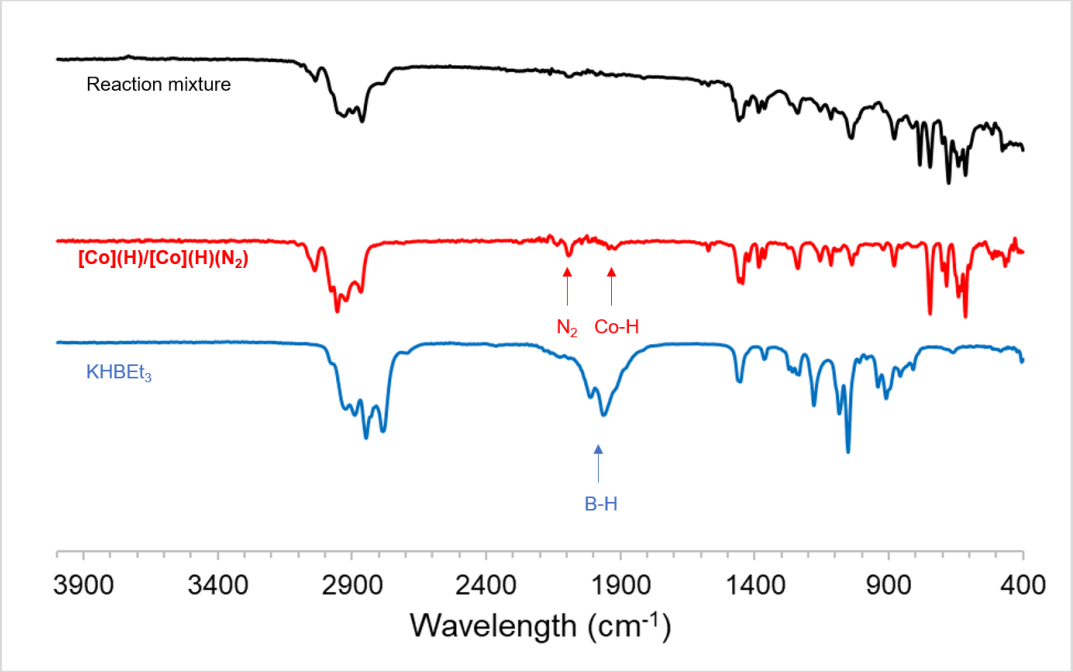


Figure S4.13 Overlay of IR spectra of the product mixture (black; thin film from THF) generated from the reaction of **[Co](D$_2$)$^{1-}$** and BEt_3, $KHBEt_3$ (blue, thin film, from THF), and independently synthesized **[Co](H)/[Co](H)(N$_2$)** (red, thin film from benzene). Peaks in the product mixture match closely with the authentic of **[Co](H)/[Co](H)(N$_2$)**. The absence of both the Co-H stretch (1943 cm^{-1}) and the B-H stretch (2014, 1955 cm^{-1}) is apparent from the product mixture, consistent with D incorporation at these positions. A simple harmonic oscillator model predicts that these resonances should shift to (1483 cm^{-1} – 1430 cm^{-1}), overlapping with stretches on the edge of the fingerprint region, complicating their unequivocal assignment.

Additional Reactions:

Control Experiments Relevant to H-atom transfer:

To confirm that the Co-H_2 adduct **[Co](H$_2$)$^{\bullet}$** does not access bimolecular HAT reactivity a solution of the complex was heated in benzene (or toluene) overnight at 60 ºC then at 80 ºC with some decomposition over the course of days, but no formation of the hydride complex **[Co](H)/[Co](H)(N$_2$)** was observed.

Similarly, heating the hydride complex **[Co](H)/[Co](H)(H$_2$)** at 80 ºC led to significant decomposition over 2 d, but does not generate **[Co](H$_2$)$^{\bullet}$**.

In the absence of H_2, $^{t}Bu_3ArO^{\bullet}$ reacts slowly with the N_2 complex **[Co](N$_2$)$^{\bullet}$** to generate unidentified paramagnetic products, but the hydride complex **[Co](H)/[Co](H)(N$_2$)** is not observed.

Control Experiments Relevant to Hydride transfer:

The anionic H_2 adduct **[Co](H$_2$)$^{1-}$** was generated *in situ* by reduction with K metal in a J. Young NMR tube in THF-d_8. After clean product formation was confirmed, the solution was frozen, the head space was evacuated and a 1:1 mixture of H_2 and D_2 was added. Examination of the resultant

^{1}H NMR spectrum confirms that this complex mediates rapid HD scrambling (spectrum shown above).

The anionic H_2 adduct **[Co](H$_2$)$^{1-}$** shows some solution stability upon mild heating (up to ~50 ºC) but decomposed rapidly upon heating to 80 ºC.

Other:
We explored conditions for the generation of the cationic dihydrogen adduct $[P_3^BCo(H_2)][BAr^F_4]$, but observed no evidence for H_2 binding to the cationic complex $[P_3^BCo][BAr^F_4]$ even at low temperatures.

5. Calculation of d_{HH} from J_{HD} and T_1(min).

Empirical correlations between J_{HD} and d_{HH} have been described by Morris[4] and Heinekey[5]:

$$d_{HH} = 1.42 - 0.0167(J_{HD})$$
$$d_{HH} = 1.44 - 0.0168(J_{HD})$$

Using these correlations to predict d_{HH} from J_{HD} = 29.5(6) Hz for the anionic H_2 adduct **[Co](H$_2$)$^{1-}$** gives a predicted distance of 0.93(1) Å and 0.94(1) Å, respectively, consistent with its formulation as a non-classical H_2 adduct. As Heinekey's equation is derived from a more rigorous data set, we cite that value in the main text.

Similarly, predicted values of d_{HH} can be derived from a corrected value of $T_{1(min\_corr)}$ that corrects for dipolar interactions with the H_2-ligated Co center and the supporting ligand (L).[6]

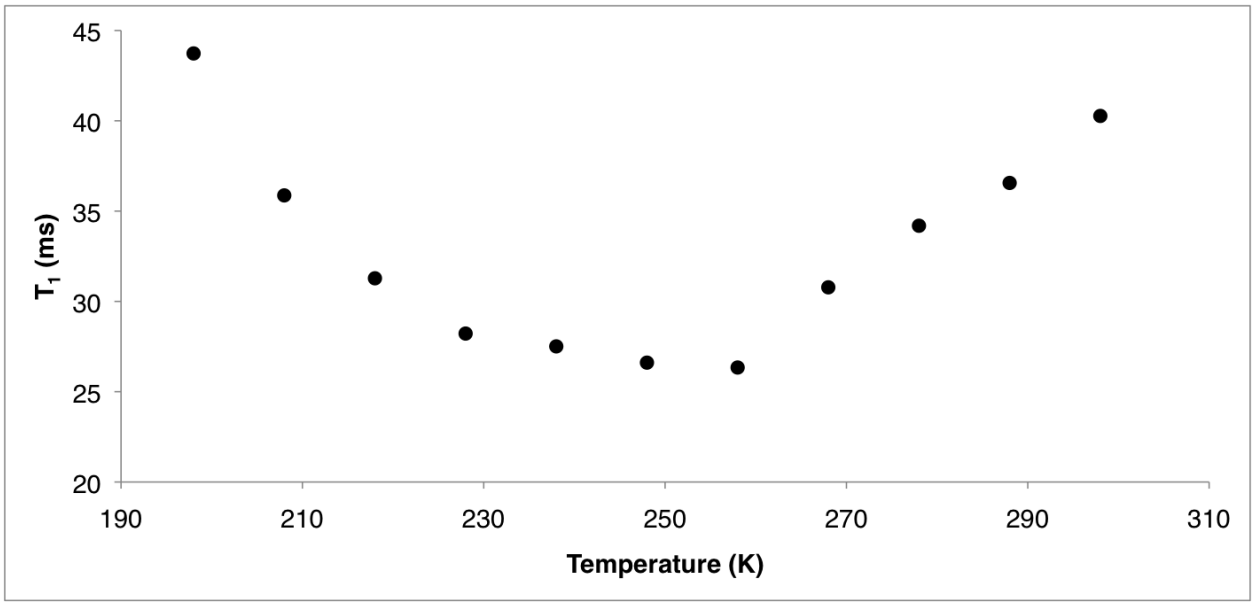


Figure S5.1. Plot of T_1 relaxation time vs. temperature as measured on a 500 MHz spectrometer in THF-d_8. A $T_{1(min)}$ value of 26(1) ms was obtained at 258 K.

A corrected value of $T_{1(min)}$, $T_{1(min\_corr)}$ can be determined from the following equation, where the dipolar interactions from the ligand and Co center can be derived from the DFT optimized structure of **[Co](H$_2$)$^{1-}$**.

(4) Maltby, P. A.; Schlaf, M.; Steinbeck, M.; Lough, A. J.; Morris, R. H.; Klooster, W. T.; Koetzle, T. F.; Srivastava, R. C. *J. Am. Chem. Soc.* **1996**, *118*, 5396.
(5) Luther, T. A.; Heinekey, D. M. *Inorg. Chem.* **1998**, *37*, 127.
(6) (a) Desrosiers, P. J.; Cai, L.; Lin, Z.; Richards, R.; Halpern, J. *J. Am. Chem. Soc.* **1991**, *113*, 4173-4184; (b) Bautista, M. T.; Earl, K. A.; Maltby, P. A.; Morris, R. H.; Schweitzer, C. T.; Sella, A., *J. Am. Chem. Soc.* **1998**, *110*, 7031-7036. (c) Vollmer, M. V.; Xie, J.; Lu, C. C. *J. Am. Chem. Soc.* **2017**, *139*, 6570.

$$1/T_{1(min\_corr)} = 1/T_{1(min)} - 1/T_1(L) - 1/T_1(M)$$

To obtain these values for the supporting ligand and metal center, the following general equation can be considered,

$$1/T_1(E) = R_E = K_X/ d^6_{EH}$$

where the parametrized corrections depend on the constant K_x, determined based on the elements gyromagnetic ratio and nuclear spin, and the distance between the nuclei of interest. Thus, for Co:

$$1/T_1(Co) = R_{Co} = 88.80\ Å^6\ s^{-1}/(1.62)^6 = 4.9\ s^{-1}$$

Similarly, for all of the protons of the supporting ligand:

$$1/T_1(L) = R_L = \Sigma\ 77.51\ Å^6 s^{-1}/\ (d_{HH})^6 = 3.9\ s^{-1}$$

A corrected $T_{1(min\_corr)}$ can then be obtained:

$$1/T_{1(min\_corr)} = 1/0.026\ s - 4.9\ s^{-1} - 3.9\ s^{-1} = 29.7\ s^{-1} = 33.7\ ms$$

From this corrected value, d_{HH} can be extracted, considering both fast and slow H_2 rotation, which has been discussed by Morris.[7]

For *slow* H_2 rotation:

$$= 1.172\ Å$$

For *fast* H_2 rotation:

$$= 0.930\ Å$$

The value derived by considering the fast rotation regime (d_{HH} = 0.93(1)) is far more similar to the value obtained from the empirical relationship between J_{HD} and d_{HH} (d_{HH} = 0.94(1)), consistent with the rapid rotation of H_2.

As shown in Table 1 of the main text, the difference between the corrected and uncorrected values of $T_{1\ min}$ is smaller for our complex than for those reported by Lu and coworkers. This is attributable to instrument normalization, with their spectra collected on a 400 MHz instrument corrected to match convention. Our spectra were obtained using a 500 MHz instrument, thus this correction was not needed.

(7) Morris, R. H. *Can. J. Chem.* **1996**, *74*, 1907.

6. IR Spectra.

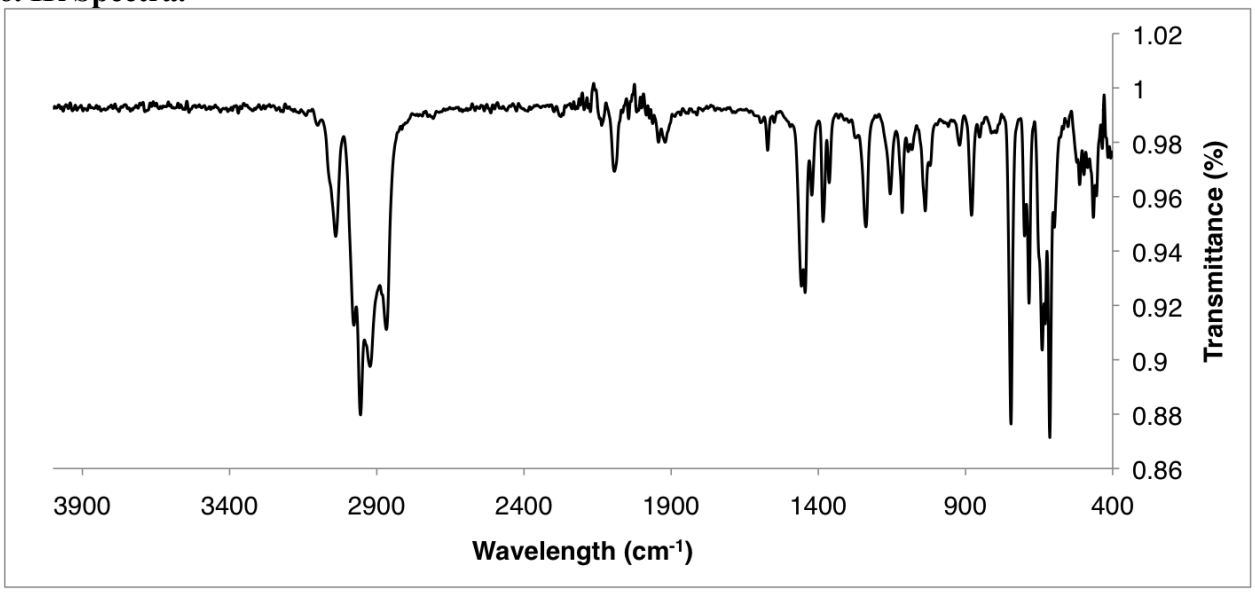


Figure S6.1. IR spectrum of $P_3^BCo(H)$ **[Co](H)/[Co](H)(N_2)** collected as a thin film under an N_2 atmosphere ($\nu_{Co\text{-}H}$ = 1943 cm^{-1}). The weak sharp stretch at 2092 cm^{-1} is reproducibly observed and may be attributable to the equilibrium N_2 ligation observed by alternative spectroscopies (UV-Vis, NMR). Alternatively, this may be due to the presence of a minor $P_3^BCo(N_2)$ impurity, with a reported N_2 stretch at 2089 cm^{-1} within the error of the instrument.

7. UV-Visible Spectra and van't Hoff Analysis of H_2 binding to $P_3^BCo(H)$.

For Van't Hoff analysis: Temperature dependent H_2 solubility in toluene[8] and toluene densities[9] were obtained from the literature.

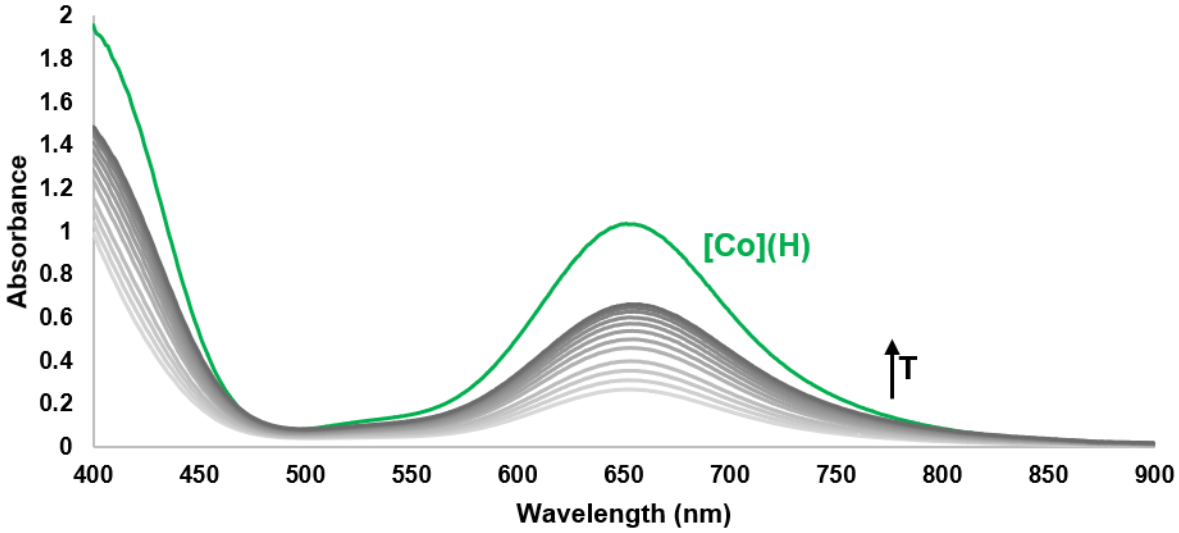


Figure S7.1. Variable temperature UV-Visible spectra of a solution of **[Co](H)/[Co(H)(H_2)** in toluene under an H_2 atmosphere, with temperature dependent behavior indicative of H_2 binding to **[Co](H)** generate **[Co](H)(H_2)** (30 – 80 °C; 5 °C increments). The green spectrum shows a sample of pure **[Co](H)** (650 nm; ε = 1440 $M^{-1}cm^{-1}$; concentration 0.72 mM) collected under vacuum in toluene.

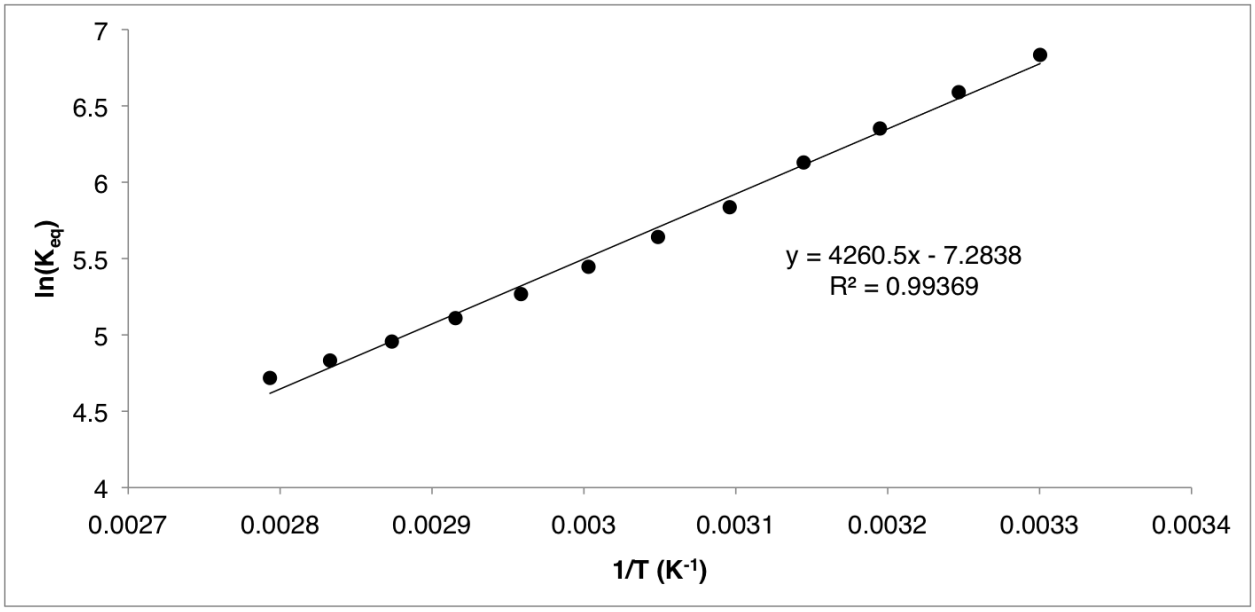


Figure S7.2. Van't Hoff plot examining H_2 binding to **[Co](H)**. This analysis gives ΔH° = -8.5(2) kcal mol^{-1} ; ΔS° = -14(1) cal mol^{-1} K^{-1}; $K_{eq}(303) = 929$ M^{-1}.

(8) Brunner, E. *J. Chem. Eng. Data* **1985**, *30*, 269.
(9) McLinden, M. O.; Splett, J. D. *J. Res. Natl. Inst. Stand. Technol.* **2008**, *113*, 29.

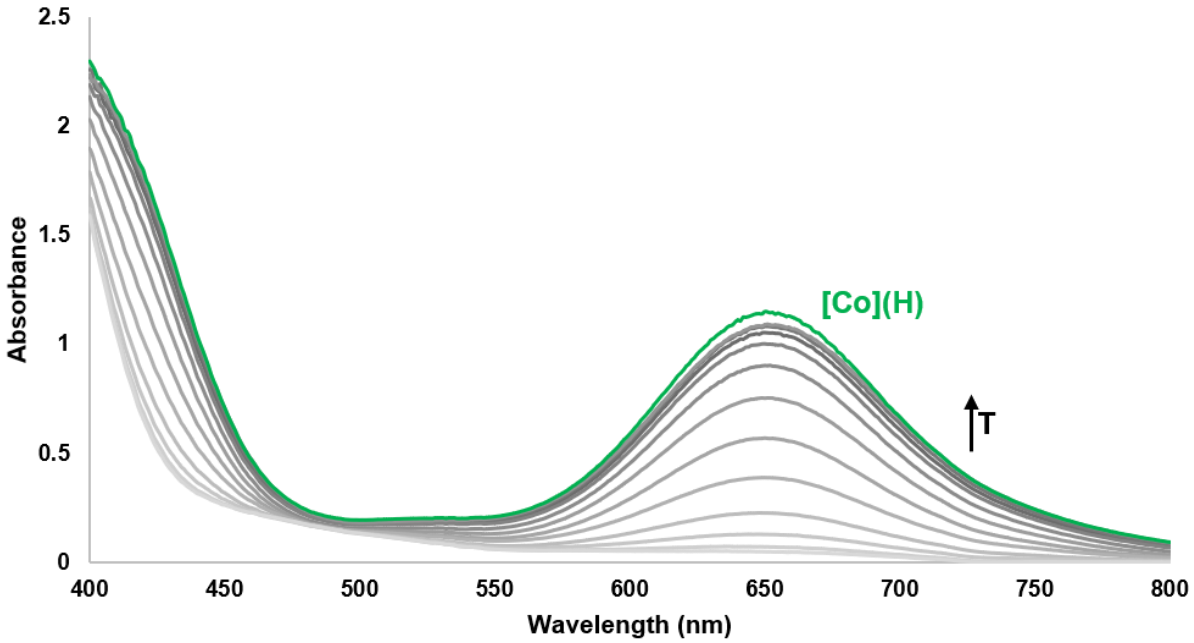


Figure S7.3. Variable temperature UV-Visible spectra of a solution of **[Co](H)/[Co(H)(N$_2$)** in toluene under an N_2 atmosphere, with temperature dependent behavior indicative of N_2 binding to **[Co](H)** generate **[Co](H)(N$_2$)** (-90 – 25 °C; 10 °C increments except 25 °C to 10 °C). The green spectrum shows a sample of pure **[Co](H)** (650 nm; ε = 1440 $M^{-1}cm^{-1}$; concentration 0.80 mM) collected under vacuum in toluene.

8. Kinetic Experiments

As noted in the main text, at both very early and very long reaction times, deviations from isosbestic behavior are observed reproducibly across independently prepared samples. The behavior at early reaction times might be attributable solution inhomogeneity, where incomplete mixing of solution phase reagents or effects of incomplete equilibration between gaseous and dissolved H_2 are problematic. An additional possibility is that a minor impurity or impurities are introduced with one of the added reagents that react competitively at early reaction times. At very long reaction times, its possible that partial decomposition of products at long times. Given the good yields of products generated through this reaction protocol, we believe interpreting the reaction that proceeds with isosbestic behavior as the reaction of interest to be reasonable.

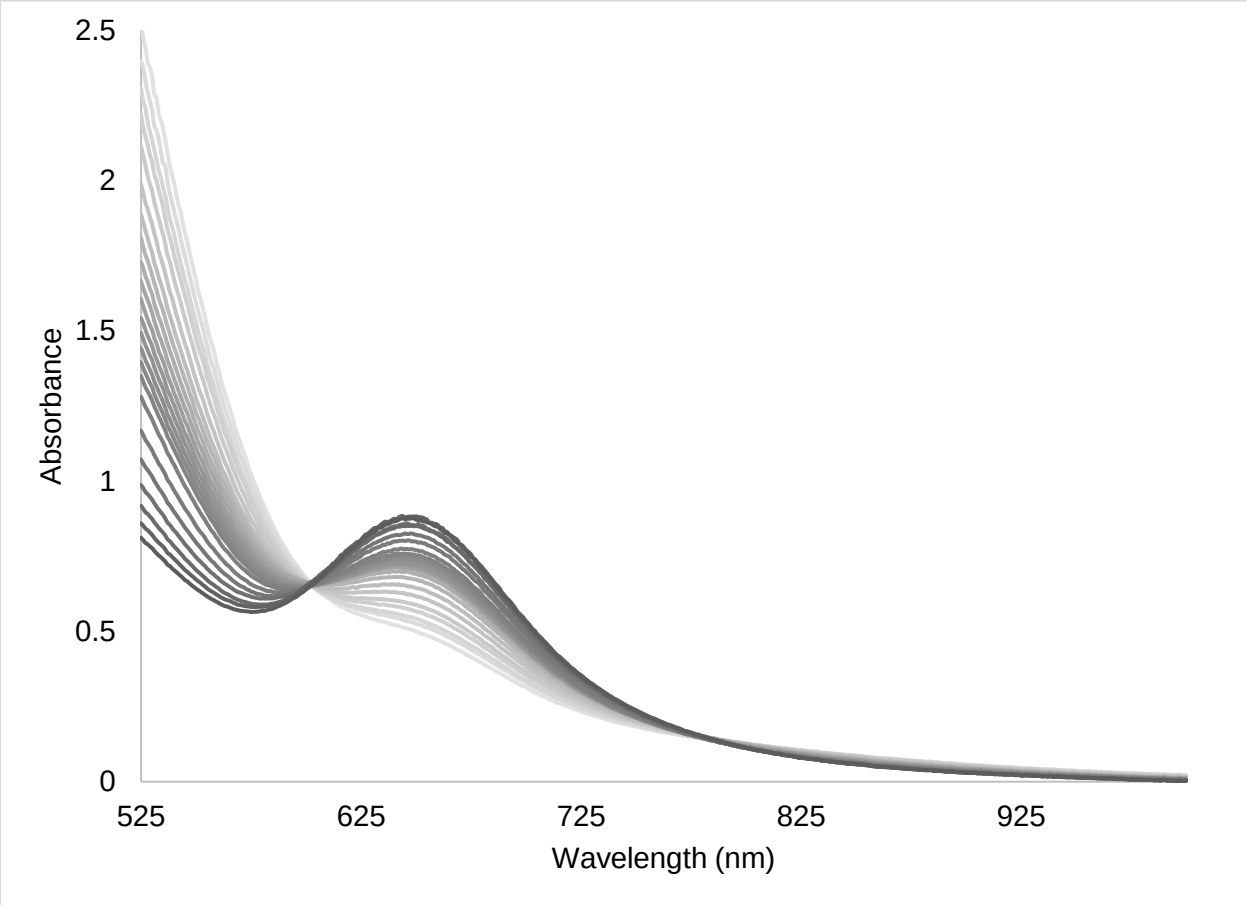


Figure S8.1. Transformation from **[Co](H$_2$)$^{1-}$** to **[Co](H)/[Co(H)(H$_2$)** at room temperature from t = 61 min to t = 1021 min monitored by UV-Visible spectroscopy. As the reaction time increases, the spectra are depicted with darker gray.

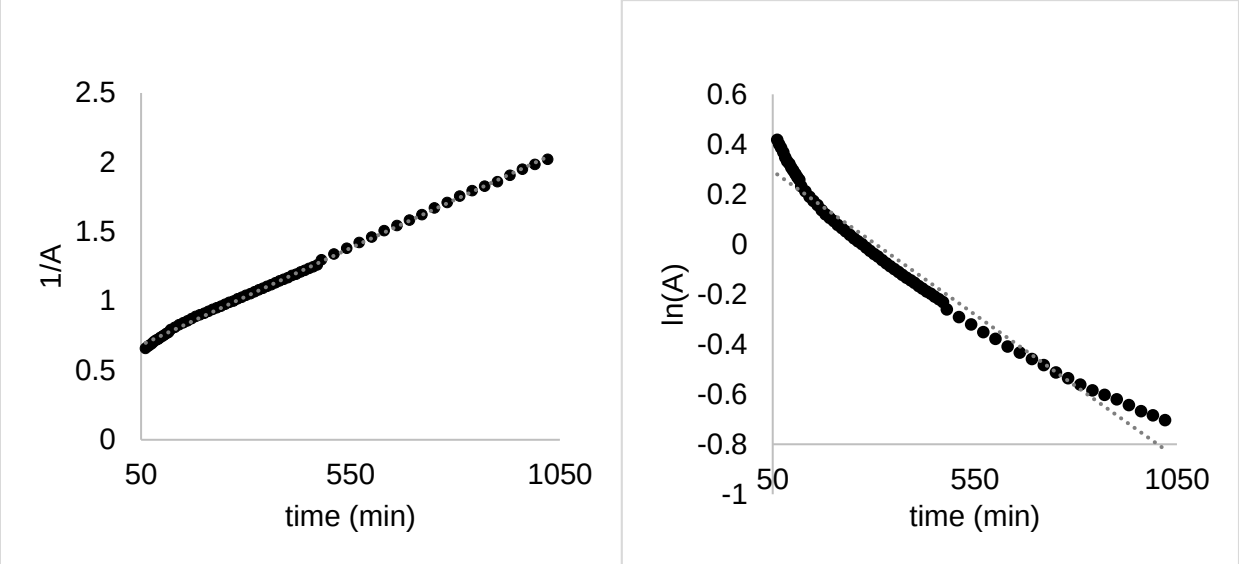


Figure S8.2. (Left) Plot of 1/A vs. t and (Right) plot of ln(A) vs. t for the reaction of **[Co](H$_2$)$^{1-}$** with BEt_3 at room temperature from t = 61 min to t = 1021 min at 550 nm.

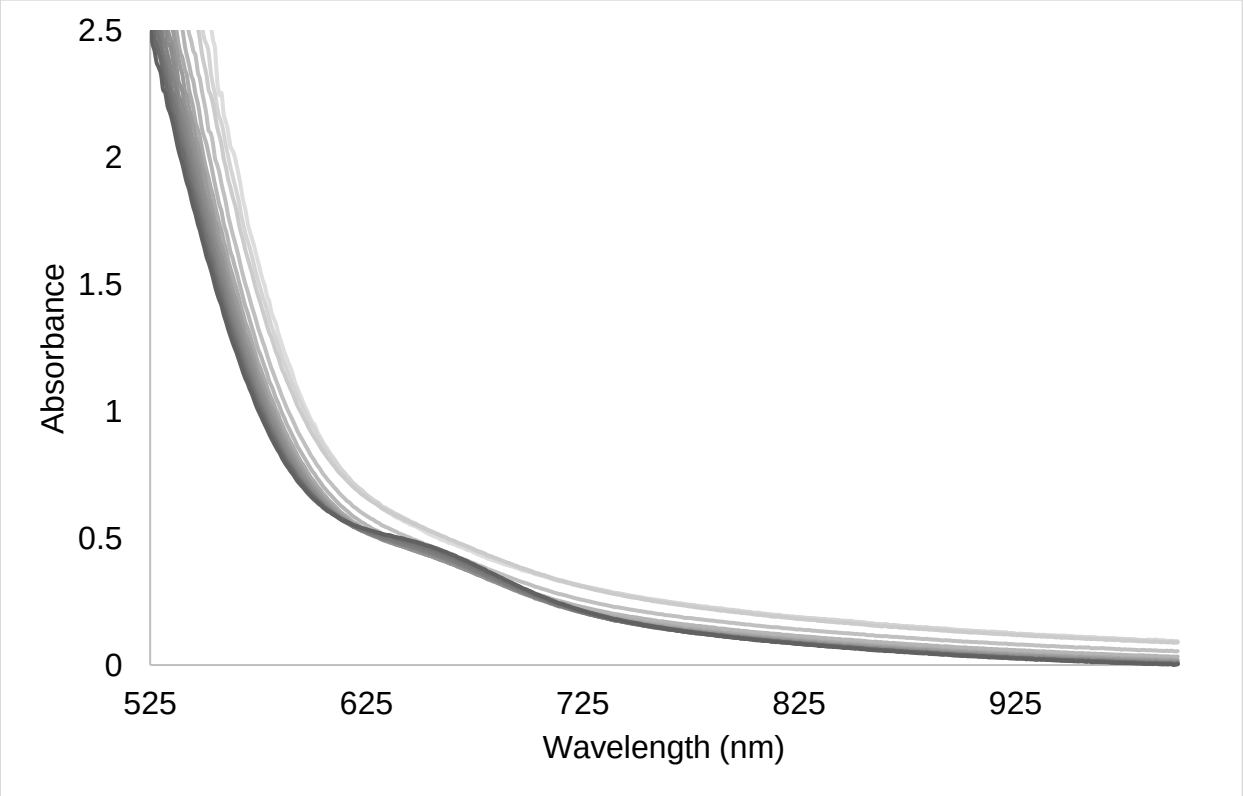


Figure S8.3. Transformation from **[Co](H$_2$)$^{1-}$** to **[Co](H)/[Co(H)(H$_2$)** at room temperature from t = 0 min to t = 61 min monitored by UV-Visible spectroscopy. As the reaction time increases, the spectra are depicted with darker gray.

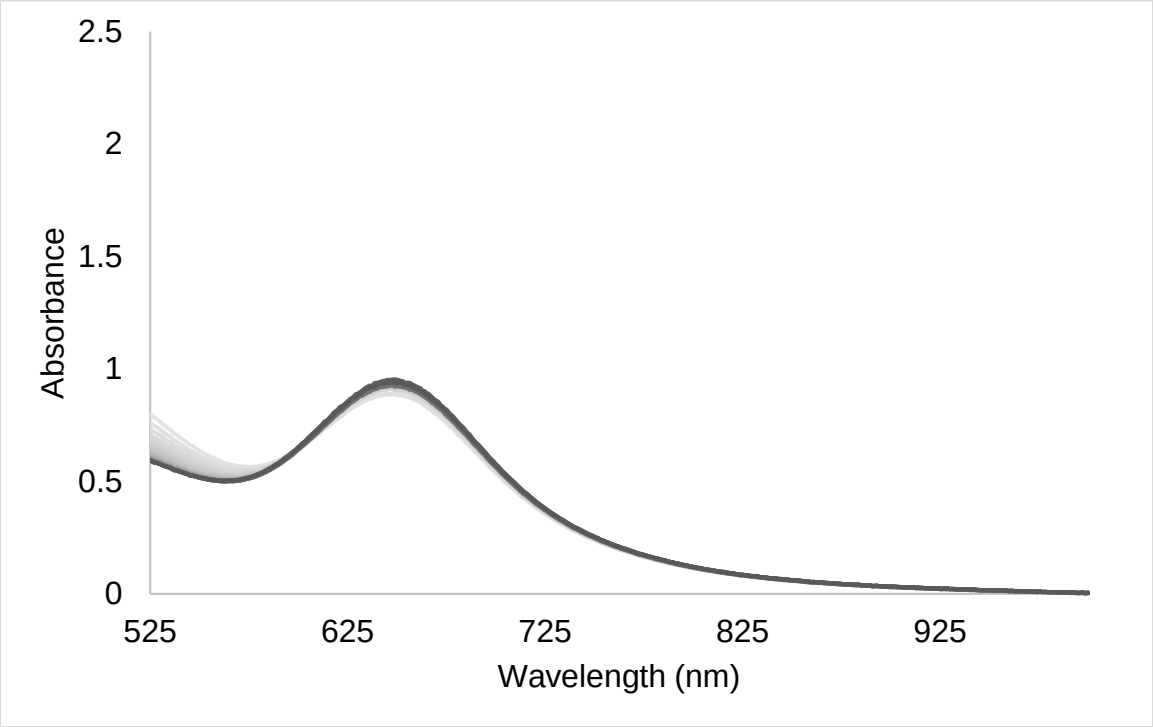
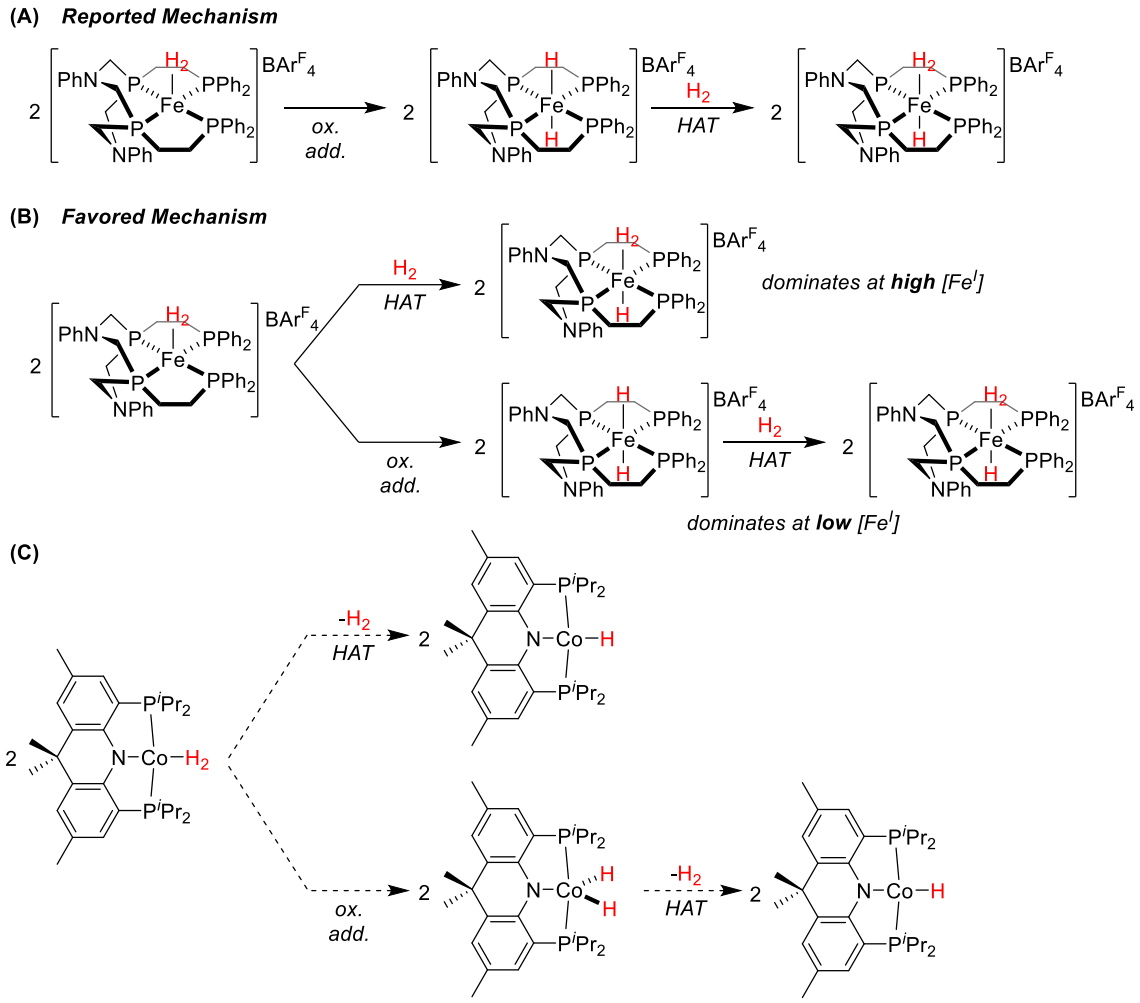


Figure S8.4. Transformation from **[Co](H$_2$)$^{1-}$** to **[Co](H)/[Co(H)(H$_2$)** at room temperature from t = 1021 min to t = 4171 min monitored by UV-Visible spectroscopy. As the reaction time increases, the spectra are depicted with darker gray.

9. Comment on Homolytic H_2 Activation by Previously Described Systems



Scheme S9.1. (**A**) Simplified representation of the reported mechanism for net bimolecular H_2 oxidative addition from an $Fe^{I}(H_2)$ adduct precursor as proposed by Bullock and coworkers. (**B**) An alternative mechanistic scenario for this transformation that is preferred based on reported experimental data. (**C**) Plausible limiting mechanisms for net bimolecular H_2 oxidative addition from a putative $Co^{I}(H_2)$ adduct precursor. No reported experimental or computational results distinguish between these possible pathways.

In a recent report from Bullock and coworkers, net bimolecular H_2 oxidative addition was reported (Scheme S9.1A) with mixed order kinetic behavior observed for H_2 activation in this system.[10] At early reaction times, the transformation is 2nd order in concentration of the Fe^{I} precursor, with a 1st order process dominating as the starting material is consumed and the reaction

(10) Prokopchuk, D. E.; Chambers, G. M.; Walter, E. D.; Mock, M. T.; Bullock, R. M. *J. Am. Chem. Soc.* **2019**, *141*, 1871-1876.

proceeds to completion. In their report, they provide a well-reasoned argument based on combined experimental and theoretical data that the observed 1st order process is the oxidative addition of H_2 at the Fe^I center to generate an $Fe^{III}(H)_2$ intermediate. They then propose that the 2nd order rate term is attributable to bimolecular HAT between this dihydride intermediate and a second $Fe^I(H_2)$ or $Fe^{III}(H)_2$ equivalent to generate two equivalents of the terminal Fe^{II} product upon facile H_2 binding (Scheme S9.1A). This sequential mechanism is inconsistent with the 2nd order term dominating the overall reaction profile at *early* times. Instead, the observed kinetics are consistent with competing 1st and 2nd order pathways, where the 2nd order reaction dominates at high Fe^I concentrations. As such, we suggest an alternative mechanism, where direct HAT from the intact H_2 adduct dominates the kinetics at high concentrations of the Fe^I precursor with a pathway proceeding *via* an initial oxidative operative as the reaction proceeds to completion (Scheme S9.1B). Alternative possible mechanisms may be considered for the second order process, for example if there is a rapid preequilibrium for deprotonation of the Fe-H_2 adduct by the pendant amines, with the 2nd order process the reaction of that hydride complex.

A second example of this reactivity pattern was reported recently by Choi and Lee, where net HAT is observed from a putative $Co^I(H_2)$ adduct precursor, where a key conclusion drawn by the authors is that the complex promotes HAT rather than simply undergoing oxidative addition (Scheme S9.1C). For the $Co^I(H_2)$ complex, reliable solution NMR characterization data could not be obtained to unequivocally assign this species because of rapid H_2 exchange. A major component of the argument provided to support its assignment and the proposed reaction pathway was the characterization of a structurally related silane σ-adduct and study of its HAT reactivity. In the solid-state, the silane complex was structurally characterized as a σ-adduct, but the solution-phase spectroscopic data provided are more consistent with a Co^{III}-silyl/hydride complex. The solution and solid-state structures of this compound are not necessarily the same. A relevant example contributed to the solution-phase misassignment of a $Co^I(H_2)/Co^{III}(H)_2$ non-classical adduct.[11] Specifically, few intact silane adducts have been reported to have such small Si-H couplings (28 Hz), and, to our knowledge, no intact adducts have been reported with Si-H ^{1}H NMR chemical

(11) (a) Bianchini, C.; Mealli, C.; Meli, A.; Bianchini, C.; Mealli, C.; Meli, A.; Peruzzini, M.; Zanobini, F. *J. Am. Chem. Soc.* **1988**, *110*, 8725−8726. (b) Heinekey, D.; Liegeois, A.; van Roon, M. *J. Am. Chem. Soc.* **1994**, *116*, 8388−8389. (c) Heinekey, D.; van Roon, M. *J. Am. Chem. Soc.* **1996**, *118*, 12134−12140.

shifts upfield of roughly -20 ppm, where the critical resonance for their complex is observed at nearly 10 ppm further upfield (-28.76 ppm).[12] It is often the case that hydrides and silane adducts fall in the same spectroscopic region and cannot reliably be distinguished simply by their ^{1}H NMR chemical shifts, but bona fide hydride ligands can fall well outside the region where reliably characterized silane adducts have previously been observed. Thus, based on the available data and literature precedent, we prefer a solution phase assignment for this species as the Co^{III} product of silane oxidative addition. Setting its uncertain assignment aside, demonstrating that this species undergoes net homolytic activation does not provide any information about the mechanism of H_2 activation, particularly with respect to the possible intermediacy of a Co^{III}-$(H)_2$ (Scheme S9.1C).

(12) (a) Corey, J. Y.; Braddock-Wilking, J. *Chem. Rev.* **1999**, *99*, 175-292. (b) Corey, J. Y. *Chem. Rev.* **2016**, *116*, 11291-11435.

10. Crystallographic Details

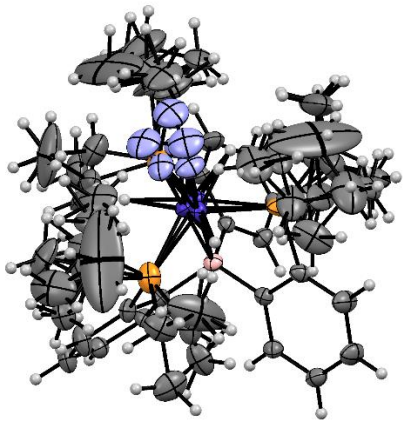


Figure S10.1. Crystal structure of the Co-H complex **[Co](H)/[Co(H)(N_2)** showing all disordered moieties.

This complex crystallizes in the absence of solvent, with the complex sitting on a three-fold symmetry axis. Detailed analysis of the bond metrics is complicated by severe disorder in the phosphorous isopropyl groups, one over two positions (79:21) and the second over three positions (30:33:36). Residual electron density associated with the hydride ligand was located in the difference map and refined freely (28% over 3 positions (86%)). Partial occupancy of an axially bound N_2 ligand is refined freely (19% over 3 positions (57%)), consistent with the observed solution phase binding of N_2 to **[Co](H)/[Co(H)(N_2)**. The level A/B alerts in the checkcif file are both associated with the large thermal ellipsoid of one of the C-atoms in the disordered isopropyl groups.

	$P_3^BCo(H)$ / $P_3^BCo(H)(N_2)$ 3/3-N_2
Crystal System	Hexagonal
Crystal size	0.27 x 0.27 x 0.29
Formula	$C_{36}H_{54.85}BCoN_{1.17}P_3$
Formula weight (g/mol)	666.81
Space group	P -3
a (Å)	11.1449(4)
b (Å)	11.1449(4)
c (Å)	16.0591(8)
α (deg)	90
β (deg)	90
γ (deg)	120
Z	2
V (Å^3)	1727.44(12)
Indep. Reflections	4540
R(int)	2.53
R1	6.01
wR2	18.74
GOF	1.04

11. Computational Methods

General considerations.

The Orca 4.0.1.2 program was used for all calculations.[13] All optimizations and energy calculations were conducted using the M06-l functional[14] and def2-TZVP basis set on cobalt with the def2-SVP basis set on all other atoms.[15] Open- and closed-shell species were modeled within the unrestricted and restricted Kohn-Sham formalisms, respectively. All geometry optimizations were conducted without symmetry constraints using gradient methods. Frequency calculations were used to confirm true minima and to determine gas phase free energy values (G_{gas}). Single point solvation calculations were done using an CPCM solvation model (Jacopo Tomasi, Benedetta Mennucci, and Roberto Cammi (2005). Chem. Rev. 105(8): 2999-3094.) with THF solvent and were used to determine solvated internal energy (E_{soln}). Solvated free energies were approximated using equation $G_{soln} \approx G_{gas} + E_{soln} - E_{gas}$. Transition states were verified by the presence of a single, large imaginary frequency that connects reactants and products. For reactions involving a change in spin state, minimum energy crossing points (MECPs) were located in addition to transition states (Harvey, J. N.; Aschi, M.; Schwarz, H.; Koch, W. (1998) Theor. Chem. Acc., 99, 95). MECP structures were verified by the absence of imaginary frequencies parallel to the crossing hyperline. Local charges and spin populations on each atom were calculated through Loewdin population analysis.

DFT Energies

Species	Free Energy (Hartrees)	ΔG (kcal/mol)
[Co](H₂)•	-3835.056247	0
[Co](H)₂•	-3835.057458	`-0.8
TS [Co](H₂)• → [Co](H)₂•	-3835.025693	19.2
OAr	-777.5500564	-
HOAr	-778.1669545	-
MECP [Co](H₂)• → [Co](H)	-4612.5974	5.6
MECP [Co](H)₂• → [Co](H)	-4612.582893	14.7
TS [Co](H₂)• → [Co](H)	-4612.56305	27.1
TS [Co](H)₂• → [Co](H)	-4612.539889	41.7
[Co](H₂)$^{1-}$	-3835.138168	0
[Co](H)₂$^{1-}$	-3835.136861	0.8
TS [Co](H₂)$^{1-}$ → [Co](H)₂$^{1-}$	-3835.125765	7.8
BEt₃	-262.1474623	-
HBEt₃	-262.82407	-
TS [Co](H₂)$^{1-}$ →[Co](H)	-4097.237484	29.4
TS [Co](H)₂$^{1-}$ →[Co](H)	-4097.245086	24.6
[Co](H)	-3834.458692	-
[Co](H₂)H	-3837.174621	0
[Co](H)₃	-3835.63046	4.3

(13) Neese, F. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2*, 73–78.
(14) Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *125*, 194101.
(15) Weigend, F.; Furche, F.; Ahlrichs, R. *J. Chem. Phys.* **2003**, *119*, 12753.

DFT Coordinates

[Co](H$_2$)$^{\bullet}$

Co	0.156492	0.186202	-1.103213
B	0.039627	0.011941	1.181329
P	0.324191	2.353946	-0.588151
P	1.624515	-1.549905	-0.764688
P	-1.997705	-0.565712	-0.947715
C	-0.499909	1.408665	1.789304
C	-1.076118	1.494373	3.068228
H	-1.169711	0.585897	3.674246
C	-1.571865	2.694099	3.574088
H	-2.029357	2.720586	4.567111
C	-1.507378	3.859503	2.809800
H	-1.914851	4.797209	3.195370
C	-0.927883	3.814095	1.543970
H	-0.893528	4.723926	0.936064
C	-0.427840	2.603963	1.047033
C	1.525512	-0.367799	1.675906
C	2.032632	0.011640	2.930142
H	1.405168	0.613644	3.597730
C	3.322584	-0.323755	3.334714
H	3.690784	-0.000516	4.312602
C	4.156818	-1.052137	2.486596
H	5.179168	-1.292924	2.788058
C	3.677889	-1.461448	1.243662
H	4.343218	-2.012991	0.572334
C	2.374428	-1.133410	0.848487
C	-0.981226	-1.207342	1.478539
C	-0.910005	-1.938377	2.677647
H	-0.134865	-1.685531	3.410666
C	-1.768228	-3.001691	2.947250
H	-1.675341	-3.555450	3.885867
C	-2.729184	-3.380070	2.009863
H	-3.386566	-4.231303	2.203616
C	-2.835966	-2.668293	0.816874
H	-3.574866	-2.982285	0.072931
C	-1.979371	-1.589927	0.559157
C	-0.489767	3.592420	-1.733275
H	-0.458950	4.568776	-1.219551
C	-1.941436	3.233631	-1.985797
H	-2.428789	3.990080	-2.619580
H	-2.517975	3.160401	-1.052714
H	-2.018412	2.265612	-2.506967
C	0.279485	3.701130	-3.040845

H	0.328639	2.727247	-3.555794
H	1.312166	4.052912	-2.909274
H	-0.217727	4.400602	-3.729605
C	2.032514	3.148286	-0.407972
H	2.537198	2.932060	-1.367653
C	1.989190	4.655706	-0.201408
H	1.437750	4.917188	0.714954
H	1.542112	5.210274	-1.036698
H	3.011488	5.043516	-0.073338
C	2.833858	2.504075	0.709127
H	3.836880	2.953984	0.767827
H	2.960317	1.423869	0.576974
H	2.350687	2.653321	1.687342
C	3.028461	-1.328891	-1.993883
H	3.886086	-1.895191	-1.591913
C	2.658258	-1.901623	-3.353093
H	1.786385	-1.381958	-3.782530
H	2.414401	-2.972989	-3.318627
H	3.486343	-1.779755	-4.067790
C	3.447232	0.127563	-2.103831
H	4.305240	0.235281	-2.784795
H	3.743369	0.545605	-1.131565
H	2.633086	0.754174	-2.504156
C	1.494719	-3.438845	-0.749580
H	0.979574	-3.676220	-1.696716
C	2.834375	-4.163052	-0.737435
H	3.396731	-3.957765	0.185312
H	3.482168	-3.931560	-1.592761
H	2.659941	-5.249865	-0.758289
C	0.642756	-3.943019	0.402773
H	0.586073	-5.042040	0.375002
H	-0.383019	-3.558890	0.382770
H	1.078766	-3.664027	1.374579
C	-2.512294	-1.733315	-2.322894
H	-3.446468	-2.219088	-1.993893
C	-2.792289	-0.950669	-3.596953
H	-1.889927	-0.424331	-3.947275
H	-3.581429	-0.195084	-3.470502
H	-3.110648	-1.620116	-4.410668
C	-1.486421	-2.826078	-2.555326
H	-1.839959	-3.539143	-3.316148
H	-1.283630	-3.395175	-1.636244
H	-0.529647	-2.411607	-2.911884
C	-3.618456	0.403086	-0.734879
H	-3.614919	1.133404	-1.561956
C	-4.886728	-0.430944	-0.848874

H	-4.925261	-1.221060	-0.083810
H	-5.027750	-0.898651	-1.832191
H	-5.764773	0.210805	-0.676787
C	-3.632765	1.168749	0.577954
H	-4.558630	1.758131	0.665643
H	-2.789459	1.860052	0.680473
H	-3.596633	0.486355	1.441905
H	0.093226	0.687378	-2.693165
H	0.245618	-0.156544	-2.738863

[Co](H)$_2^{\bullet}$

Co	0.139797	0.201231	-1.237069
B	0.039528	-0.004778	1.436040
P	0.191195	2.385516	-0.706336
P	1.679294	-1.517107	-0.820461
P	-1.974615	-0.603567	-0.991287
C	-0.410386	1.474308	1.913003
C	-0.870204	1.696607	3.220099
H	-0.876273	0.859363	3.927295
C	-1.361219	2.929230	3.643696
H	-1.719502	3.053736	4.668980
C	-1.413410	3.995475	2.750148
H	-1.811335	4.963875	3.062538
C	-0.957885	3.815893	1.446148
H	-1.014976	4.658703	0.751036
C	-0.454509	2.578625	1.018124
C	1.514052	-0.538337	1.844473
C	2.049390	-0.342272	3.124857
H	1.435442	0.154094	3.885078
C	3.351614	-0.713939	3.453325
H	3.737247	-0.531901	4.460086
C	4.169341	-1.290899	2.485751
H	5.201663	-1.561472	2.720187
C	3.663000	-1.514363	1.206937
H	4.323674	-1.950684	0.452636
C	2.346250	-1.161318	0.877028
C	-1.088705	-1.149388	1.589002
C	-1.165270	-1.830963	2.815981
H	-0.478864	-1.549631	3.622775
C	-2.047144	-2.885736	3.033783
H	-2.063625	-3.395425	4.000937
C	-2.884907	-3.310468	2.004832
H	-3.559737	-4.157426	2.150912
C	-2.850271	-2.645630	0.782176
H	-3.501280	-2.992860	-0.025440
C	-1.979193	-1.566042	0.571307

C	-0.648626	3.661991	-1.768386
H	-0.558169	4.639130	-1.263808
C	-2.118761	3.340420	-1.955312
H	-2.619310	4.126371	-2.540616
H	-2.653300	3.245993	-0.998580
H	-2.233323	2.394341	-2.507012
C	0.068067	3.728914	-3.110475
H	0.069860	2.742012	-3.599837
H	1.113804	4.056004	-3.024099
H	-0.439053	4.434706	-3.785169
C	1.916809	3.132320	-0.516009
H	2.419709	2.899547	-1.472047
C	1.926064	4.638964	-0.307757
H	1.366393	4.922868	0.597118
H	1.515927	5.205902	-1.154123
H	2.959520	4.988707	-0.160872
C	2.676106	2.446822	0.607663
H	3.726119	2.776563	0.620836
H	2.673557	1.353895	0.518650
H	2.243269	2.689251	1.590532
C	3.123009	-1.284988	-1.984682
H	3.959288	-1.901057	-1.613185
C	2.726005	-1.772096	-3.371298
H	1.878018	-1.185918	-3.759508
H	2.431270	-2.831653	-3.387541
H	3.561819	-1.656160	-4.077687
C	3.578038	0.162616	-2.022788
H	4.413519	0.287826	-2.728130
H	3.919961	0.515960	-1.039819
H	2.761029	0.821669	-2.360981
C	1.539453	-3.405896	-0.784171
H	0.999596	-3.645540	-1.715408
C	2.865046	-4.152833	-0.803563
H	3.463216	-3.949970	0.096900
H	3.484462	-3.940497	-1.684880
H	2.669818	-5.236388	-0.808506
C	0.704145	-3.875057	0.395968
H	0.574678	-4.967437	0.357361
H	-0.294247	-3.424287	0.424056
H	1.194649	-3.637482	1.353038
C	-2.464183	-1.791514	-2.345155
H	-3.398394	-2.286581	-2.029995
C	-2.724506	-1.014276	-3.628009
H	-1.815885	-0.479598	-3.946399
H	-3.526138	-0.268512	-3.523927
H	-3.015755	-1.693013	-4.443951

C	-1.410512	-2.860802	-2.555270
H	-1.728658	-3.576426	-3.329018
H	-1.220029	-3.431071	-1.633946
H	-0.460442	-2.410733	-2.884550
C	-3.593723	0.365636	-0.785374
H	-3.570669	1.109324	-1.598704
C	-4.862884	-0.460056	-0.937661
H	-4.919771	-1.264059	-0.188227
H	-4.985191	-0.908525	-1.932319
H	-5.740722	0.183349	-0.770277
C	-3.624740	1.105055	0.542852
H	-4.504133	1.765778	0.592630
H	-2.736126	1.723202	0.712294
H	-3.693999	0.404431	1.389869
H	0.371853	0.294658	0.281759
H	0.095857	0.266329	-2.748390

TS [Co](H$_2$)$^\bullet$ → [Co](H)$_2^\bullet$

Co	0.033628	-0.113381	-1.055158
B	-0.018643	-0.251064	1.275473
P	0.469348	2.136273	-0.675203
P	1.869575	-1.225150	-0.942442
P	-2.157662	-0.567357	-0.812087
C	-0.502046	1.231927	1.713142
C	-1.107913	1.392257	2.972747
H	-1.245579	0.513788	3.613109
C	-1.578303	2.625137	3.418746
H	-2.052687	2.705331	4.400618
C	-1.474201	3.749529	2.601874
H	-1.871644	4.712838	2.930499
C	-0.867492	3.629722	1.353896
H	-0.808084	4.507279	0.703035
C	-0.376401	2.391893	0.918760
C	1.500420	-0.587241	1.684759
C	1.918978	-0.401998	3.013906
H	1.196526	-0.046647	3.757274
C	3.237132	-0.613391	3.412247
H	3.526276	-0.444309	4.453035
C	4.192649	-1.017900	2.481495
H	5.232176	-1.165646	2.783618
C	3.811037	-1.221265	1.157451
H	4.565463	-1.521027	0.423021
C	2.483629	-1.012319	0.762769
C	-1.140782	-1.340342	1.630881
C	-1.111028	-2.103257	2.807485
H	-0.273629	-1.980331	3.503867

C	-2.103610	-3.036574	3.103074
H	-2.045546	-3.624526	4.023102
C	-3.158378	-3.236006	2.215381
H	-3.927663	-3.982222	2.428100
C	-3.216822	-2.488015	1.039736
H	-4.029216	-2.677014	0.332281
C	-2.225744	-1.543994	0.748618
C	-0.312035	3.300716	-1.910062
H	-0.272298	4.311712	-1.470149
C	-1.764438	2.957854	-2.169288
H	-2.215702	3.679627	-2.867259
H	-2.356839	2.976311	-1.243306
H	-1.859101	1.955556	-2.615926
C	0.503069	3.283648	-3.195440
H	0.522575	2.271605	-3.632371
H	1.545963	3.599712	-3.046251
H	0.063959	3.957324	-3.946598
C	2.107067	3.041524	-0.349611
H	2.742402	2.792027	-1.213153
C	2.000088	4.558603	-0.276926
H	1.345301	4.887902	0.543309
H	1.651217	5.027656	-1.206244
H	2.994502	4.981281	-0.065832
C	2.779819	2.519691	0.910033
H	3.761185	3.000373	1.043360
H	2.941139	1.436240	0.894440
H	2.182100	2.744514	1.807403
C	3.300128	-0.894458	-2.097680
H	4.135484	-1.526742	-1.750402
C	2.920302	-1.293403	-3.516285
H	2.066638	-0.694476	-3.869905
H	2.632143	-2.349824	-3.608632
H	3.759651	-1.119974	-4.206555
C	3.743176	0.552512	-2.050704
H	4.639136	0.707238	-2.670942
H	3.983259	0.886221	-1.030635
H	2.952984	1.205152	-2.451657
C	1.731179	-3.102221	-1.077685
H	1.164538	-3.262790	-2.012612
C	3.073741	-3.813491	-1.178804
H	3.707456	-3.602492	-0.302915
H	3.645742	-3.561625	-2.080814
H	2.918277	-4.902627	-1.195641
C	0.937506	-3.697919	0.076884
H	0.806740	-4.779772	-0.075887
H	-0.064501	-3.265674	0.196118

H	1.462619	-3.563409	1.035663
C	-2.752882	-1.772663	-2.115616
H	-3.741263	-2.116580	-1.767719
C	-2.920817	-1.054418	-3.445747
H	-1.950888	-0.668069	-3.797657
H	-3.616028	-0.203226	-3.389121
H	-3.306074	-1.738864	-4.216744
C	-1.866352	-2.995431	-2.250701
H	-2.305567	-3.706626	-2.967114
H	-1.740670	-3.525060	-1.294874
H	-0.869019	-2.718851	-2.622245
C	-3.710990	0.531032	-0.670120
H	-3.623130	1.223591	-1.522934
C	-5.050130	-0.182955	-0.803308
H	-5.209628	-0.921280	-0.003976
H	-5.198388	-0.681828	-1.769565
H	-5.861163	0.555638	-0.704897
C	-3.703911	1.344314	0.614381
H	-4.593775	1.991426	0.659510
H	-2.824971	1.990216	0.711960
H	-3.730137	0.693792	1.502923
H	-0.031712	-0.695259	-2.479325
H	-0.160241	-1.470999	-0.528958

OAr

O	-0.44468073094877	0.33576471968886	-4.72623394845542
C	-0.58150452906831	0.20381158364270	-5.95917217729784
C	0.58840291565388	0.10899972908587	-6.85103398331004
C	2.04614950691174	0.16286212298314	-6.37134554598893
C	0.38121413127662	-0.03960331839078	-8.21418564325587
H	1.25386482297547	-0.11090151572221	-8.86587583226787
C	-0.89161056845380	-0.10273662989576	-8.79918489377488
C	-1.11200580199464	-0.26770819107028	-10.30009463018359
C	-2.00826749638571	-0.00925494963616	-7.94467976224718
H	-3.00149190199752	-0.05711045389149	-8.40039316189554
C	-1.92029411140783	0.13687991124630	-6.57558501789889
C	-3.24066273242375	0.22170802266022	-5.79391645308356
C	2.26017716752620	0.33216507261155	-4.86708866735197
C	2.74511042738970	1.34272287943856	-7.06733642995869
C	2.74518564609182	-1.14160356838507	-6.78913972520629
C	-3.12107228958006	0.37126812925005	-4.27707775121724
C	-4.04867554657537	-1.05798644641838	-6.06477860973728
C	-4.03280639255454	1.43271150172073	-6.31323274200768
H	-3.51439721190976	-1.94913253318198	-5.70438735472108

H	-4.26395173693253	-1.20908131832934	-7.13213135258933
H	-5.01478522143939	-1.01633831173554	-5.53970420941514
H	-2.59546228940900	-0.46937356484893	-3.80988929946520
H	-4.13690530495132	0.41470464730653	-3.85403770603179
H	-2.59231648876129	1.28474618952231	-3.98247132956510
H	-3.48739625237811	2.37074040650718	-6.13405570613849
H	-4.99964808426496	1.50728311796478	-5.79309280877210
H	-4.24475562367567	1.37243658551820	-7.39026041121938
H	2.27682270158744	-2.01499637404587	-6.31239987492445
H	3.80130614106944	-1.12077687245669	-6.48131196942467
H	2.72451035868395	-1.30566471953322	-7.87581153794406
H	1.82799820773230	1.26240459701761	-4.48123491056697
H	3.34431536777002	0.35570028894261	-4.67499151735222
H	1.83079189056072	-0.48999660599434	-4.28364939116396
C	0.20013918964957	-0.35168192659296	-11.07558737833662
C	-1.91183399991243	0.93173124936351	-10.82619823721567
C	-1.90885008710334	-1.55494930496630	-10.55183450634126
H	-1.36478319902357	-2.44002922170241	-10.19151395124542
H	-2.09200332102099	-1.68896739128219	-11.62856495096755
H	-2.88793546996670	-1.54244114395531	-10.05240584632885
H	0.80907952926380	0.55662850114634	-10.95926081737497
H	-0.00387538924105	-0.47062930977945	-12.14921445629302
H	0.81136890943406	-1.21115976605421	-10.76403375205476
H	-1.37012610352671	1.87537845810437	-10.66721079820351
H	-2.89145581123200	1.02586641058478	-10.33671448265718
H	-2.09437191155937	0.82748203718723	-11.90630554209289
H	2.27678733919301	2.29991117827259	-6.79545597644947
H	2.72496571235285	1.26279200095270	-8.16337842603605
H	3.80115564257594	1.39040409715013	-6.76231652397001

HOAr

O	-0.52733199352018	0.35179927053819	-4.64081712550694
C	-0.59479990647109	0.20324717607386	-5.99137332027178
C	0.55504462820912	0.11429175478444	-6.81257323554206
C	2.03965407127458	0.16271789218384	-6.36959424345120
C	0.35780679790597	-0.03655813492380	-8.19400172529017
H	1.24382952533886	-0.10547192000402	-8.82667631529769
C	-0.89481729585255	-0.10187889792617	-8.79029760649849
C	-1.10934203047634	-0.26812277742568	-10.29556559424939
C	-1.99375436109538	-0.00893434992317	-7.93530216531340
H	-2.99457687109221	-0.05592388266771	-8.37260131824296
C	-1.89571784933583	0.14056498782498	-6.55304451462516
C	-3.23384505641989	0.22422212631309	-5.78365401437301
C	2.31232314589957	0.32719034202883	-4.86934023801536
C	2.72808163346098	1.34665514398127	-7.06517376113554
C	2.72713130960186	-1.14441094771950	-6.79189802852026

C	-3.14892126159523	0.37381430237376	-4.26257981696166
C	-4.03545407635311	-1.05719287569281	-6.05955322742091
C	-4.02047254850258	1.43523814112911	-6.30797466963594
H	-3.49950611163574	-1.94561457294686	-5.69429837027991
H	-4.23852644445807	-1.21219600403046	-7.12838104072027
H	-5.00761557250583	-1.02064533292291	-5.54450552008444
H	-2.63578451400961	-0.46777202463812	-3.78313413387015
H	-4.17338756493737	0.41281360406026	-3.86129316613807
H	-2.63642531985729	1.29259889343695	-3.95563747257938
H	-3.47433659996510	2.37192348316449	-6.12275736515734
H	-4.99371195796815	1.51181126856196	-5.79929004883742
H	-4.21947158069732	1.37875791489181	-7.38737964296679
H	2.26340639480358	-2.01440601315842	-6.30433783094483
H	3.79198033960905	-1.13148358603204	-6.51240601185827
H	2.67700171511538	-1.31259312334473	-7.87561255565179
H	1.93474031655165	1.27892531557247	-4.46399633324578
H	3.39813190599623	0.34537849265412	-4.69858586102018
H	1.93369966108501	-0.51360245567363	-4.26737948567330
C	0.21126380658233	-0.34817361031033	-11.05743612859386
C	-1.90598605377968	0.92783130345973	-10.83049501477720
C	-1.89828640007089	-1.55688135189421	-10.55627429950528
H	-1.35358792512982	-2.43955931184785	-10.19017063981307
H	-2.07892681502507	-1.69653475437704	-11.63334313148662
H	-2.87873429779723	-1.54677333374013	-10.05847052724946
H	0.81640037471275	0.56198246985563	-10.93185927283225
H	0.02319509418463	-0.46781268033573	-12.13436449238006
H	0.82188133608687	-1.20529827399738	-10.73674281509306
H	-1.36686781457505	1.87237579079560	-10.66613209879450
H	-2.88678949562876	1.02054947093254	-10.34207408809325
H	-2.08673979026778	0.82800232800556	-11.91194644828658
H	2.26542245778925	2.30212080173029	-6.77763797400352
H	2.67791665552338	1.27619832751155	-8.15958087175926
H	3.79298127461830	1.39346637302042	-6.78958056235558
H	0.39139506467384	0.38367324064795	-4.36574587559648

MECP [Co](H$_2$)$^{\bullet}$ → [Co](H)

Co	0.45251056827932	-0.29318375812522	-1.32643457098594
B	0.08970587124469	0.33240772015146	0.80585996075624
P	0.58785809888886	1.91761923099048	-1.55840300643237
P	1.86176474240194	-1.73140314496717	-0.22722258876223
P	-1.66323862562511	-1.08442631370075	-1.17475681127253
C	-0.46695027816879	1.85439136906096	0.89542502608728
C	-1.18834604712881	2.36076578084369	1.99032331842263
H	-1.42355766232229	1.69748406240804	2.83065107290440
C	-1.61909616549816	3.68480505314269	2.03923212405356
H	-2.17852277993672	4.04542331940420	2.90736296777148

C	-1.34430187856113	4.55611644783226	0.98349910974880
H	-1.68453065253332	5.59411486606156	1.01957832968154
C	-0.65135975085126	4.08144997145835	-0.12707210132904
H	-0.45111618336621	4.75751755574291	-0.96552232185954
C	-0.24059062855079	2.74270773792745	-0.17089696062854
C	1.49511974120298	0.20403408309682	1.61039265975003
C	1.84905687135333	1.00250194263860	2.71140820968107
H	1.14199462016815	1.75766031020786	3.07270606836850
C	3.09494421923936	0.90140732144274	3.32758781015681
H	3.34306716045803	1.55568202035223	4.16859329863345
C	4.03946660689575	-0.01193092126788	2.85973924606230
H	5.02856182738496	-0.07288854501851	3.32065170985884
C	3.71084254961633	-0.84261685865289	1.79037285900255
H	4.45715906853156	-1.54949409960416	1.41477478100234
C	2.45244759712092	-0.73955623290254	1.18362570596791
C	-1.00194881554554	-0.70134968677072	1.42391773244318
C	-1.12272416352126	-0.90407929513631	2.81031487183014
H	-0.44540797134841	-0.36876749108810	3.48655466000170
C	-2.04735702234692	-1.79250851347034	3.35344011765708
H	-2.10402281040103	-1.92953664988505	4.43726063136581
C	-2.89763787831739	-2.51604036067308	2.51648887171889
H	-3.61493606094695	-3.22677138438985	2.93468139163241
C	-2.81943734546444	-2.32584066511546	1.13894533914372
H	-3.47423708744289	-2.90820713564879	0.48260164357291
C	-1.88786453640221	-1.42729894690587	0.60123419128868
C	-0.11328854924531	2.78830604591206	-3.06899365619348
H	0.11292667944771	3.85875235211058	-2.92865171527326
C	-1.61627907689715	2.63846984729214	-3.18477436870174
H	-1.98422588886996	3.12907166975875	-4.10151385832576
H	-2.15217901975475	3.08264628568723	-2.33495355584740
H	-1.89836373788267	1.57643104713196	-3.24326425962050
C	0.56721442459584	2.30568468400298	-4.33242482418831
H	0.32231039594394	1.24711911263284	-4.52766812875664
H	1.66609686619238	2.38576751255731	-4.30543960202345
H	0.21644859469564	2.87822221781421	-5.20458431909760
C	2.33281718720214	2.67401069686840	-1.58320914612103
H	2.87576260100717	2.07347335885588	-2.33630632239215
C	2.39373939311566	4.13956187917677	-1.99415940304706
H	1.77704023324001	4.77207646073789	-1.33591100603323
H	2.08523465319629	4.32674772304417	-3.03184733803947
H	3.42748619431811	4.50712855302420	-1.90126051642604
C	3.02443207205605	2.49311249604203	-0.24297454445037
H	4.05521837583586	2.87776881104455	-0.28888147388754
H	3.07357025126580	1.44574235136618	0.07286494256791
H	2.50304341023663	3.04355314439772	0.55586969545104
C	3.37856023633371	-1.99971214348280	-1.30503894837364

H	4.18506119500974	-2.34777008213335	-0.63733050216368
C	3.11124590820574	-3.07287485317249	-2.34851375949014
H	2.25070516513266	-2.80658771044787	-2.98519250259665
H	2.89568576581085	-4.05614884226426	-1.90727978687764
H	3.97827521410526	-3.19889961381043	-3.01592284686744
C	3.83738425364293	-0.70221261073511	-1.94638469365411
H	4.73904518972402	-0.86393944534481	-2.55869689799192
H	4.07792246487759	0.06387435878780	-1.19593016862920
H	3.06096613015938	-0.28760938379279	-2.60985489005381
C	1.70092547536879	-3.47050610980808	0.51703316351702
H	1.32056503544391	-4.08723934335627	-0.31418793741852
C	3.01588767026612	-4.07222642442621	0.99495616709959
H	3.44161425805501	-3.49932909415007	1.83175686828596
H	3.78408371737322	-4.16392207407100	0.21620864700782
H	2.83113522653094	-5.08839177031027	1.37657935659979
C	0.69489879132836	-3.51414230245822	1.65436578967885
H	0.63332893714237	-4.53522309941129	2.06146802906070
H	-0.31540545883202	-3.21698995352352	1.35269891321898
H	0.99668284999651	-2.85198542318589	2.48074781001883
C	-2.00271767936777	-2.72458750194913	-2.02596051572304
H	-2.96426293401905	-3.09409788696464	-1.62934493392760
C	-2.14185627049854	-2.53097778941760	-3.52682210238857
H	-1.23993718169322	-2.07168723872775	-3.96277052895060
H	-2.99611506514532	-1.89283566076694	-3.79138113997085
H	-2.28802899618832	-3.49353631266257	-4.04085992083525
C	-0.94338882501215	-3.75938801088672	-1.70419673897960
H	-1.19453402261478	-4.73051881538448	-2.15847447583717
H	-0.84267980733883	-3.91538361202406	-0.62107381892295
H	0.04155459721946	-3.45795278304441	-2.09609493980199
C	-3.25901121009675	-0.16721090901987	-1.61717315223558
H	-3.10760945517982	0.14128647303828	-2.66823274898605
C	-4.53591098515047	-0.99106512554411	-1.55195111997954
H	-4.71402645665476	-1.37968550967341	-0.53753646004484
H	-4.55567266139788	-1.83893031531363	-2.25042305262222
H	-5.40154962960032	-0.35607923409677	-1.79912029842771
C	-3.40120243163207	1.07875534392313	-0.75911269093986
H	-4.24098671394675	1.70063764289244	-1.10711613329072
H	-2.49802521377825	1.70069281334774	-0.76206532680641
H	-3.59978781797807	0.81354579751934	0.29126459369890
H	0.55831693477096	-0.40114245223182	-2.97969799312905
H	0.76576567641043	-1.18942810603863	-2.69571507306219
O	-0.79891794657764	-1.20182542440429	-6.62117733540383
C	-0.44588369902465	-0.07906949530147	-7.01934177732289
C	0.98627087565398	0.23386295517117	-7.21948872530596
C	1.32773740656811	1.50957297097551	-7.59823317219800
H	2.38182522232163	1.76602338732851	-7.71465592892349

C	0.37545605377192	2.53670666804643	-7.80872768841753
C	0.87087768135482	3.93570835942079	-8.15784523928589
C	-0.99471016894619	2.22832011526565	-7.67005056749860
H	-1.72208797294183	3.01944412802567	-7.84516375756680
C	-1.44483650782021	0.97937936034382	-7.29160007538495
C	-2.93107759215804	0.67069006922073	-7.14631433031882
C	-3.24035761058370	0.39683478359302	-5.66692797448573
C	-3.31123943256716	-0.54509340904191	-8.00750131904890
C	-3.80201932437860	1.84490416095466	-7.59343829433493
H	-3.63809748884405	2.74650205961395	-6.98514484583469
H	-4.86212221686529	1.57697909978592	-7.48455674229993
H	-3.63890325867131	2.11045372707304	-8.64873438864008
H	-2.53616453043299	-0.31547311811480	-5.22428244050912
H	-4.25659642584573	-0.01240985603725	-5.55720725152038
H	-3.19779215518246	1.32587877742888	-5.08126992524704
H	-2.83752321154717	-1.46633656548174	-7.65434389575961
H	-3.02777098140614	-0.39163500563019	-9.05962027381015
H	-4.40132604989247	-0.68819661665882	-7.97986912408868
C	2.03731100057380	-0.83468001731474	-6.95071295278165
C	1.98802688619905	-1.26193639469063	-5.47530739336316
C	3.44869655350232	-0.31485281817517	-7.22911098980017
C	1.79258832404649	-2.05105450393371	-7.85679393406446
H	2.15748411475085	-0.40211960415354	-4.80948726899074
H	2.78581418196078	-1.99169577249778	-5.27424333760742
H	1.02924238957185	-1.72163300094649	-5.20648977352602
H	0.82418747256720	-2.52265540468720	-7.65749941105003
H	2.57771873173091	-2.80264119027435	-7.68840082578801
H	1.82975539225132	-1.76888676094498	-8.91952280032619
H	3.71617677278600	0.53330374380726	-6.58058609852437
H	3.58404380369506	-0.00122116708746	-8.27487726745468
H	4.17964026220456	-1.11150989921533	-7.03378371813682
C	-0.26729389291630	4.94451247712001	-8.28861764837406
C	1.62687759947516	3.86237587872723	-9.49277572868768
C	1.82869986636249	4.42682991473796	-7.06240559641107
H	-0.96481785312161	4.68630904223696	-9.09803108049750
H	0.13843955517371	5.93977369255926	-8.51709722995416
H	-0.84618529925706	5.03673409444818	-7.35786555707391
H	0.97801221116043	3.50111541136172	-10.30341669751454
H	2.49858189786275	3.19534923532358	-9.44099019655723
H	1.99366243875309	4.85968041973785	-9.77633960115419
H	1.31608003595463	4.54044708839782	-6.09628636871204
H	2.23924170762317	5.40974919144062	-7.33553052208818
H	2.68023304611579	3.74901528767080	-6.90818811445170

MECP [Co](H)$_2^{\bullet}$ → [Co](H)

Co	-0.08478528783217	-0.07302112563195	-0.98677419858953

B	0.25454285265013	-0.13775308779876	1.67748370867850
P	0.01909949263822	2.14380633551083	-0.59743536924313
P	1.48307212935745	-1.79051512956510	-0.72600027090335
P	-2.13784181980330	-0.83071110708354	-0.33736718406227
C	-0.11323515101534	1.36769336279988	2.13895003040701
C	-0.34013844936506	1.66146792463588	3.49253932532864
H	-0.22161431889303	0.86171603308184	4.23246463731258
C	-0.76483416476656	2.91405407865733	3.92838114663415
H	-0.94654311063755	3.09316016786417	4.99143239665908
C	-0.97932512705234	3.92977187531733	3.00081796289588
H	-1.33038878256741	4.91294114760081	3.32332509402547
C	-0.74518539827099	3.68136832707028	1.65059331964663
H	-0.93125174695261	4.48492312712528	0.93241955109444
C	-0.30516765168761	2.42493468368524	1.20745291668573
C	1.77890127714645	-0.65479749645364	1.86317979646673
C	2.52991310314872	-0.37807613661663	3.01365503861756
H	2.05784944033456	0.17508448200725	3.83354554086794
C	3.87063918678737	-0.73876574254824	3.13330610492723
H	4.42698886330610	-0.49020841134114	4.04111736821911
C	4.50745338353899	-1.38856209353588	2.07982346947356
H	5.56583005322521	-1.65172717780443	2.14725255058905
C	3.78546960801249	-1.69262339392972	0.92743383943238
H	4.30505791751973	-2.18377881483165	0.09999080461008
C	2.43097884000410	-1.34830274459151	0.80964820011667
C	-0.82856061628924	-1.27044156508899	2.07425758915607
C	-0.69659675404400	-1.89867448814591	3.32451874509850
H	0.11451374471403	-1.58566323135311	3.99206001320841
C	-1.52761934336275	-2.93865186085607	3.73227426276297
H	-1.38065451325457	-3.40604071454509	4.70966829998868
C	-2.52677116846818	-3.40244426615278	2.87890191176525
H	-3.16587652583731	-4.23832902012111	3.17382848743327
C	-2.69936003227892	-2.79123130499581	1.64006603836200
H	-3.47707182505379	-3.16651073150803	0.96805063990863
C	-1.87514372598880	-1.72945579344199	1.23861047404692
C	-1.00644193479400	3.38550648031332	-1.53251428609015
H	-0.84708780608306	4.37104133276610	-1.06268804269473
C	-2.48339066871404	3.04770072943965	-1.47446526661061
H	-3.07742749127575	3.81878343757682	-1.98836537807322
H	-2.86065106057045	2.96799884430290	-0.44419215610509
H	-2.67227661268553	2.09351298109216	-1.99006912525995
C	-0.52487263571691	3.43997705253243	-2.97402356291701
H	-0.60715404755848	2.45481509615756	-3.45872129690703
H	0.51975135147255	3.77084828352950	-3.06337355829371
H	-1.13871096837931	4.14455475875949	-3.55666852521506
C	1.74978262429530	2.87548390977782	-0.77227271665888
H	2.04882563106614	2.60518247975330	-1.80245757417216

C	1.81552036119940	4.38700339672321	-0.61997716038703
H	1.45761944842846	4.70560720705045	0.37138682645517
H	1.24239272959372	4.93354190179250	-1.38102278548508
H	2.85971539663034	4.72629436904038	-0.70199831060578
C	2.70566190355831	2.20616158664311	0.20146420229525
H	3.74362625180536	2.51143246441463	-0.00126871644539
H	2.66497231841194	1.11060330688862	0.14891961596107
H	2.47760389258099	2.48533417158840	1.24190047189143
C	2.72489393835048	-1.67830314422452	-2.11726805426703
H	3.57964945105779	-2.32452495095402	-1.85717903756543
C	2.08027746981169	-2.20690734374414	-3.39058663530086
H	1.24286857318120	-1.55926494128932	-3.70082574983647
H	1.68320376860179	-3.22653063708829	-3.28060768734535
H	2.81319421815596	-2.23379267026076	-4.21109880100307
C	3.24071543283434	-0.26274732896079	-2.30115621784065
H	3.89999106704339	-0.20049923339765	-3.18123632544182
H	3.81583458120315	0.08341116549390	-1.43052827243010
H	2.41010353229207	0.44345696313668	-2.46590203918019
C	1.32501716473684	-3.67430912128089	-0.54628475344497
H	0.63811592116924	-3.95738980848911	-1.36155021091518
C	2.61939938028026	-4.45360357095370	-0.72978235134483
H	3.36315915839465	-4.20261520658242	0.04066118218752
H	3.08529633185121	-4.32202651012353	-1.71505919018116
H	2.41125986822881	-5.52932354304298	-0.62134935716768
C	0.68625494125404	-4.05623779556390	0.77854104925540
H	0.55889013737739	-5.14818540084318	0.83491365894567
H	-0.29847118830626	-3.60099415320556	0.92700202800847
H	1.31649597804729	-3.75690976468819	1.63067995176035
C	-2.86491918245271	-2.03684814043420	-1.56156754639144
H	-3.75334634659970	-2.50060740326904	-1.10085360353465
C	-3.28366340529807	-1.24083933911194	-2.78789246387682
H	-2.40920582804860	-0.72703169191161	-3.21953995125474
H	-4.04011536384841	-0.47321038185891	-2.56580873437115
H	-3.70485967362862	-1.89230124480273	-3.57012616873002
C	-1.88782728828426	-3.13636250951712	-1.92644649479199
H	-2.33829432990157	-3.83572859328341	-2.64767992195555
H	-1.58500496485263	-3.71997319143363	-1.04507269684586
H	-0.98173185001352	-2.71321176336869	-2.38960424828637
C	-3.69107455003556	0.16358488479741	0.11688532807752
H	-3.80477254905957	0.88145565220531	-0.71099710961673
C	-4.97447602522992	-0.64810915221099	0.21335546857792
H	-4.90740966995701	-1.43354240098229	0.98149753969072
H	-5.27575357313393	-1.11730138761045	-0.73236303369612
H	-5.80227602567032	0.01211405991299	0.51596187641788
C	-3.48519478209240	0.94395769305241	1.40528002130969
H	-4.33696806399530	1.61874684664308	1.58338563506263

H	-2.57556291911477	1.55444777089909	1.39688638064237
H	-3.41306852603486	0.27201776273605	2.27498460180007
H	0.38252315541333	0.08759745692884	0.47127909906773
O	-0.84325486567249	1.02844974887901	-5.31612478244269
C	-0.74716207743539	0.82774491013048	-6.54205932882616
C	0.56726772139602	0.77218558243900	-7.20779548204059
C	1.89225123656717	1.15929988611558	-6.53731967947947
C	0.63096344505210	0.29318909200679	-8.50672351207599
H	1.61296006572965	0.18407588275971	-8.97014625377793
C	-0.50357975921401	-0.04846797294159	-9.25765972360982
C	-0.42351699069569	-0.61603040368291	-10.67020419460869
C	-1.76708491270172	0.16306981881948	-8.66851260758368
H	-2.65305373591419	-0.04543429959679	-9.27474915410636
C	-1.94474891164169	0.60474348195821	-7.37413880946721
C	-3.38538709715116	0.84605829855900	-6.89799043724548
H	-0.36952544430085	-0.08856343405141	-2.47296435904303
C	1.77199743513869	1.80911723604388	-5.15908063745752
C	2.62217533605404	2.16596114278258	-7.44215117887078
C	2.75321767960218	-0.10390004285795	-6.40213783925604
C	-3.54521172571509	1.27315894640762	-5.43894208340485
C	-4.19602073116276	-0.44806223127511	-7.07387495293734
C	-3.99346386120826	1.94644074117705	-7.78190143302900
H	-3.76951825538398	-1.26567378445386	-6.47431168229213
H	-4.23993314360889	-0.78851386737470	-8.11778667280158
H	-5.23258419763441	-0.29567525780157	-6.73730299914983
H	-3.20954327571842	0.47776132051090	-4.76534356750476
H	-4.61386086954005	1.45783478092088	-5.24683877607817
H	-2.98885338640998	2.18503782134741	-5.18900622688258
H	-3.44670435314153	2.89413492701843	-7.66939808846992
H	-5.03978444145715	2.13058754819993	-7.49491436752898
H	-3.98484629449391	1.68384217710689	-8.84954912827708
H	2.24435747579299	-0.86051472934196	-5.78977877776925
H	3.71184867248287	0.13367674572852	-5.91521668957831
H	2.98150987674878	-0.55979322083264	-7.37640059748565
H	1.13408941635650	2.70197544589890	-5.18770824678186
H	2.77587352489961	2.12375299490483	-4.83034649193892
H	1.35559491327219	1.13786229389507	-4.39859587880776
C	1.01631767720150	-0.78734206987871	-11.14633141842666
C	-1.14938991329578	0.32848720512753	-11.63669671016846
C	-1.10897520328530	-1.98903449617665	-10.68922700383894
H	-0.61260855655086	-2.69291265097584	-10.00550640144332
H	-1.07447370596983	-2.42277028494814	-11.69987197631235
H	-2.16575037613137	-1.93023035000864	-10.39271436983614
H	1.55739675578153	0.16918335220016	-11.18555204378707
H	1.03036650684752	-1.20997890140168	-12.16093747145886
H	1.58628753665987	-1.47156365931410	-10.50098069976499

H	-0.68432053763702	1.32488153527617	-11.64695846131571
H	-2.20845629540418	0.45983838470880	-11.37388310906195
H	-1.11349167296182	-0.06879194611197	-12.66212426349492
H	2.03291498148627	3.08529254502077	-7.57365225294746
H	2.84261801505363	1.76645928917137	-8.44160540469744
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TS [Co](H$_2$)$^{\bullet}$ → [Co](H)

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P	2.00950796918222	-1.70937311357897	0.14089135338156
P	-1.52200543586561	-1.18403915020749	-0.99665878966048
C	-0.50522042607881	1.82665810370558	1.14924027991561
C	-1.32203238484446	2.30379400251142	2.18880006260908
H	-1.63101084364386	1.61656568759508	2.98401811163518
C	-1.77281108041514	3.62109332805136	2.22537057678000
H	-2.41961229669045	3.95425384561981	3.04185828608230
C	-1.40790895893112	4.51749209983481	1.22061397306954
H	-1.76600014678107	5.54965393376099	1.24103283858668
C	-0.59974361400116	4.07673352599630	0.17640243039563
H	-0.34565521650417	4.76949679882850	-0.63225952799727
C	-0.16311818219519	2.74599698805569	0.13957502483433
C	1.45936328243651	0.22792531340751	1.95536087533011
C	1.74191186162433	1.06625790783425	3.04744050214508
H	0.99391794527847	1.80371240094712	3.35959455628805
C	2.96055193694782	1.01650418452563	3.72029360433685
H	3.15048283767574	1.69515961654561	4.55660597949730
C	3.95009873776866	0.12174743556366	3.31469417629849
H	4.92013889537098	0.10162529356231	3.81725466379010
C	3.69490102565254	-0.73941340753949	2.24949348710728
H	4.48174281398244	-1.42333088948110	1.91791379746052
C	2.46164223269300	-0.69464226815520	1.58732477893154
C	-1.01006312236223	-0.75399313843870	1.64997153888828
C	-1.16494981065444	-0.99216588644719	3.02774206848787
H	-0.50672543868861	-0.47173938058774	3.73304811425238
C	-2.10398427845286	-1.89214451745791	3.52363724671548
H	-2.18704135443622	-2.06008001731979	4.60109159075041
C	-2.92346044557271	-2.59877108036817	2.64422533226623
H	-3.65161934410300	-3.32078295065724	3.02209582036158
C	-2.79266085578389	-2.38997625425082	1.27387254342700
H	-3.42133201379951	-2.96930110299330	0.59139477668462
C	-1.84868310456986	-1.47928772156985	0.77851881209577
C	0.09974226113155	2.90455670702383	-2.73611130416209
H	0.35571171118253	3.95950030964549	-2.54448999180226
C	-1.40838465738483	2.83119042227320	-2.86736945936206

H	-1.74132970775506	3.39273776232684	-3.75347877919506
H	-1.91787582992942	3.26286609576774	-1.99596629483227
H	-1.75698458506800	1.79413300070111	-2.97988615203594
C	0.82223257383231	2.45512469781437	-3.99486675178193
H	0.59484598138579	1.40265245901378	-4.22579724269458
H	1.91607831168927	2.55053951074453	-3.91483828926599
H	0.50652098742332	3.05255759446326	-4.86467666562995
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H	3.05540383046866	2.12119738931095	-1.91396905059338
C	2.59108291302392	4.18093770584387	-1.56004265150530
H	1.92799212424001	4.81126550359475	-0.94750599095513
H	2.37819933220072	4.38061085783651	-2.61811818631001
H	3.61703968701181	4.53553309281566	-1.37590203914321
C	3.12277033964097	2.51854183871368	0.19473938571346
H	4.19339382895513	2.77384376400882	0.16222026194368
H	3.03322256792929	1.49530180587387	0.56916604229461
H	2.65165491956107	3.17501178777526	0.94311793328255
C	3.61536610417505	-1.90943097970092	-0.81386777039693
H	4.38565322610258	-2.21544326092248	-0.08655944444954
C	3.45997876574083	-3.00014391360105	-1.85950051228658
H	2.58886324067459	-2.79888029438482	-2.50168950450698
H	3.31931104751980	-3.99819452626149	-1.42134159094030
H	4.34288435445965	-3.05424578076084	-2.51671158292776
C	4.06153649967413	-0.59648850989327	-1.43258126973311
H	4.97484139223509	-0.73961604419627	-2.03125178522111
H	4.28442135679642	0.16163962774736	-0.66961589841800
H	3.29422713317982	-0.18253592935575	-2.10693515352341
C	1.86589751670528	-3.44837400692807	0.88778513283035
H	1.58844432614232	-4.08624418955212	0.03158944141606
C	3.16590946133887	-3.98887124929522	1.46746328758126
H	3.52945435209154	-3.37047770907064	2.30052953500281
H	3.97672520324869	-4.09240934392518	0.73404337876101
H	2.98669344103901	-4.99341757294911	1.88146106357743
C	0.78049865882753	-3.53480102952784	1.94739673382050
H	0.65981166287290	-4.57772309625684	2.27904641480616
H	-0.19719864188967	-3.18012332571596	1.60631111492094
H	1.04588755779987	-2.93797235190542	2.83405235198914
C	-1.80420903228631	-2.89252837020193	-1.74429990782971
H	-2.72575491430982	-3.27101709301682	-1.26851651057312
C	-2.02465764489477	-2.88032960459689	-3.24379212038700
H	-1.18498398968056	-2.41823375200464	-3.78007492229206
H	-2.93314553607783	-2.34397367149231	-3.53580359428685
H	-2.12531616889589	-3.91062325344901	-3.62111038809021
C	-0.67682250375483	-3.83995772990254	-1.38590475503191
H	-0.87511366347575	-4.84881789762978	-1.78065004398275
H	-0.54884097979237	-3.92933488539686	-0.30073754712185

H	0.27995105297228	-3.49941903743984	-1.81622006538162
C	-3.07434248912762	-0.27924418797902	-1.56896570998228
H	-2.85236842715726	-0.01068574229324	-2.62102661104684
C	-4.36966119076058	-1.07813492821270	-1.52448346847812
H	-4.64430692177313	-1.32917796817698	-0.48869484316104
H	-4.35087627802980	-2.01084837156199	-2.10244242657238
H	-5.19585518108526	-0.47105440225341	-1.92788578264894
C	-3.24532565563040	1.00019063383951	-0.76523644645220
H	-4.01246363476646	1.64845873318530	-1.21680252889752
H	-2.31796003929783	1.57987997776657	-0.69120783450100
H	-3.56406542280840	0.77571854806667	0.26451721008336
H	0.77613933839165	-0.35229303830706	-2.68058628632319
H	0.97692064455544	-1.14128966516873	-2.40429955139724
O	-0.33258107350672	-0.59569670133569	-4.85793310447799
C	-0.16668926972172	-0.69200418647327	-6.09728138521536
C	1.05940243341397	-1.29195356403303	-6.66866690731545
C	1.23327668635867	-1.30568869602934	-8.03633748364256
H	2.14966640712401	-1.73118147257940	-8.44640915063311
C	0.28322955896795	-0.81278009915382	-8.95222158206944
C	0.58397645170334	-0.87463533585344	-10.44582817283291
C	-0.91304146177974	-0.30064924562811	-8.42912009054269
H	-1.66648054603518	0.05617924718439	-9.12897407307886
C	-1.18261726994359	-0.22466060823686	-7.07224481606274
C	-2.51497748829813	0.35640092367102	-6.60547296733103
C	-2.23374071352129	1.65569700425227	-5.85006017642988
C	-3.21756885386416	-0.63464983392236	-5.67268885706315
C	-3.46610080170569	0.66851435549614	-7.76045537012979
H	-3.07280866478126	1.43759910545572	-8.44119214996774
H	-4.41155005631433	1.05610971510825	-7.35513257548984
H	-3.70959630974666	-0.22277866848698	-8.35793048027238
H	-1.52968780042376	1.47387974178899	-5.03426609304269
H	-3.16160293945139	2.06443701806612	-5.41989521688774
H	-1.80224687276710	2.42036635008746	-6.51453591513343
H	-2.59507258055236	-0.83021621169997	-4.79692889740356
H	-3.40954441010692	-1.59341223734537	-6.17870699856238
H	-4.18535011508525	-0.23057324729908	-5.33754059742555
C	2.12244736004740	-1.90971660459102	-5.76392105439934
C	2.77746523161157	-0.82376044606108	-4.90022781617910
C	3.24466367036946	-2.57544020734460	-6.56582644415751
C	1.47952268367298	-3.00896713814744	-4.90595189695875
H	3.23028590166166	-0.04662097625389	-5.53508100157771
H	3.58605768254085	-1.25689793473180	-4.29152821610812
H	2.06965126851836	-0.33396102943235	-4.22175087606317
H	0.79439702032081	-2.60976491013066	-4.14815163610716
H	2.25631476683009	-3.59714904000204	-4.39898535246302
H	0.90505373331009	-3.70676169156461	-5.53498320882306

H	3.80529362642152	-1.86074267266135	-7.18583195248828
H	2.87566681764228	-3.37925802457002	-7.22017196537307
H	3.96613190009024	-3.02853792333984	-5.87083666388400
C	-0.54906670857264	-0.29988565627015	-11.29216725194549
C	0.80428461072860	-2.33811828182932	-10.85440328863427
C	1.86188537663578	-0.07375956573353	-10.73268601176971
H	-1.49005909780227	-0.85220623827917	-11.15604070112996
H	-0.28999538762610	-0.35888272787417	-12.35888272297545
H	-0.74207138283791	0.75797778485037	-11.06215900761546
H	-0.09293543142201	-2.94594068909515	-10.66801666758592
H	1.63818580151016	-2.80165598533700	-10.30878828451693
H	1.03760625403923	-2.40602498488894	-11.92765508651255
H	1.74609184813152	0.98213617775804	-10.44845139517771
H	2.10298686494360	-0.10716023397046	-11.80582446607028
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TS [Co](H)$_2$$^{\bullet}$ → [Co](H)

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P	1.70070700323530	-1.86103860563445	-0.47179515574363
P	-1.97392400932157	-1.05864798340925	-0.38175657763879
C	-0.17444610118368	1.17825918163407	2.39601418972813
C	-0.47735758802640	1.38990775860880	3.75085594350408
H	-0.41445010396756	0.54390141175515	4.44358830432859
C	-0.89221945417211	2.62205560379182	4.24612993247216
H	-1.12870953414780	2.73790846825857	5.30708807706729
C	-1.01870935289945	3.70107794849379	3.37676818105236
H	-1.35161578861046	4.67564796308074	3.74186319562532
C	-0.72647922251430	3.52839407952131	2.02715779563819
H	-0.84255378901450	4.38932318463003	1.36554521130030
C	-0.30725613604036	2.28765611991635	1.51917342653484
C	1.75141915689939	-0.77167788728761	2.15412708912189
C	2.39844434820515	-0.50108398641049	3.36825353269898
H	1.83110276024077	-0.02112688307903	4.17336578775058
C	3.75525514275416	-0.75029296020695	3.56285963210734
H	4.22937920713640	-0.49637179132764	4.51469050188835
C	4.51295157416150	-1.28596893854497	2.52518279327662
H	5.58536732401457	-1.45555801383526	2.64846600822345
C	3.89106599638818	-1.60660340377211	1.32081415117947
H	4.49994678666301	-2.02591473256905	0.51516183239356
C	2.52047093805295	-1.38151063335008	1.12973911948474
C	-0.89245779281587	-1.42564266692830	2.16361831240435
C	-0.87843813210367	-2.03035809355841	3.43332876248511
H	-0.10822890571438	-1.73041113514700	4.15299648183697
C	-1.77149115399824	-3.03278698852362	3.79988861343370

H	-1.71248324649873	-3.48220646433229	4.79476450143516
C	-2.72350630641164	-3.47924410071789	2.88553513594314
H	-3.41647448236416	-4.28172112880975	3.14996335087660
C	-2.77435212913362	-2.89703612107090	1.62298920193359
H	-3.51105860851563	-3.26482838809015	0.90225142078604
C	-1.88221953940673	-1.87734066920474	1.25899445941059
C	-0.92758528431141	3.47378149092371	-1.10680512505687
H	-0.73918226604639	4.38011772493458	-0.50929587589659
C	-2.41953926495684	3.20484260444629	-1.09133377275574
H	-2.96176727052466	4.04063995049004	-1.56056113351633
H	-2.81665365185256	3.08469026902064	-0.07318427935938
H	-2.66956251994958	2.30331243817154	-1.66825179235690
C	-0.43335781923931	3.70630971592363	-2.52558929929869
H	-0.51751078627746	2.78040068997869	-3.10798427654643
H	0.61196402953841	4.04200395949322	-2.56904122618365
H	-1.04262065116687	4.47889258166219	-3.02025886583633
C	1.80176527897275	2.81797155848623	-0.40535438878033
H	2.06579769042859	2.69934872420877	-1.47354607744975
C	1.91480976405969	4.29039550002372	-0.03738840031674
H	1.59893762390441	4.47130251671528	1.00171888396316
H	1.33697161600728	4.95769261330451	-0.69012924414559
H	2.96595083050351	4.61040663461471	-0.10843985668912
C	2.75799931055287	1.99349677920313	0.43544068216711
H	3.79705839428122	2.32684628098063	0.29034832532212
H	2.71402054958807	0.92599567794898	0.18924118649190
H	2.52859979526559	2.08526056501523	1.50890690598480
C	3.06257181221564	-1.83881456744615	-1.75148656760179
H	3.84780684875241	-2.52660911395800	-1.39770183502462
C	2.51075910595304	-2.37955035002949	-3.06231778407264
H	1.72147431345003	-1.71892207606304	-3.45955911096634
H	2.07818349977733	-3.38570182298882	-2.96455108279329
H	3.30837485947727	-2.44741239462073	-3.81701143780609
C	3.70841106911646	-0.47490998250297	-1.91543339171566
H	4.50422159635908	-0.52070606925905	-2.67594500653913
H	4.17652195749573	-0.12719140521971	-0.98391659799509
H	3.00188689965079	0.30222409918592	-2.24574312324960
C	1.59276779211126	-3.74567222309700	-0.15498915977848
H	1.44568029263715	-4.17468356465804	-1.16198415925372
C	2.87019345289267	-4.37375664812004	0.39786718419391
H	3.06410153705161	-4.06577475954104	1.43396223850782
H	3.77479045314356	-4.17694162715739	-0.19347339042599
H	2.74348335796265	-5.46737445108693	0.41251676330328
C	0.47010184249228	-4.12935631094617	0.78868458123976
H	0.45284244996012	-5.22152264285533	0.92492905829776
H	-0.52425147453823	-3.81716344374352	0.46472169079299
H	0.63603037463135	-3.68627752901443	1.78276491869711

C	-2.50204594392383	-2.35416150003313	-1.63021948900881
H	-3.36062753237593	-2.89694230893219	-1.19544655367470
C	-2.95135116361863	-1.68184787444732	-2.92047975017040
H	-2.14706326600677	-1.06026102293121	-3.34760905623370
H	-3.83383561262902	-1.04199336739241	-2.78932439815241
H	-3.21657235599665	-2.44370054286480	-3.67012661450038
C	-1.40997653959406	-3.36034358945194	-1.94166028299885
H	-1.75875331865279	-4.07729390559871	-2.70100359968830
H	-1.11023749724851	-3.94194718565059	-1.06311110422564
H	-0.51638672561394	-2.85555323679142	-2.34301823197589
C	-3.57437607205090	-0.07236419914071	-0.17389551917264
H	-3.58384794302357	0.59600535612484	-1.05222105598430
C	-4.87184997470644	-0.87103007144177	-0.14579014142895
H	-4.91642700782567	-1.53308759047020	0.73251055406084
H	-5.05247395404593	-1.48122521981612	-1.03800363661477
H	-5.72517505750036	-0.18074439206867	-0.05486228433442
C	-3.48719752222509	0.79649125314898	1.07186873436686
H	-4.31507794699361	1.52168608575662	1.09875102682976
H	-2.54682790364390	1.36074098839408	1.13603892882685
H	-3.55398457488210	0.18567619053982	1.98493182223027
H	0.45098457042587	0.00455840729778	0.69734993540222
O	-0.57998316394570	1.16580625117251	-4.36107698370561
C	-0.56257206192229	0.69026262665017	-5.51179765921518
C	0.70167302384357	0.41316245672165	-6.21423344742508
C	2.04453003613844	1.03875950142054	-5.81670171382481
C	0.66553284910199	-0.39736456628046	-7.33826776053216
H	1.60788338027095	-0.64560086207087	-7.82973184366486
C	-0.52685407631042	-0.89300136632570	-7.89064428118364
C	-0.55843554386814	-1.82810447053542	-9.09612522005641
C	-1.74326920860968	-0.45253495139009	-7.32723716563086
H	-2.67126424412858	-0.74454271467982	-7.82654106633021
C	-1.81676874750553	0.35696508287041	-6.21293829879653
C	-3.17955679061537	0.95047664073062	-5.83132174519505
H	-0.16166756334962	-0.15272443804719	-2.27621368927703
C	2.05749288441253	1.75023147704575	-4.46262875180136
C	2.38832011536564	2.07322444419845	-6.90227236124191
C	3.14638830842869	-0.02807676553610	-5.78054291438706
C	-3.24911951760641	1.64457090877398	-4.46810760171365
C	-4.26609517892819	-0.13188970005005	-5.87197261902038
C	-3.50385602321523	2.00680279753407	-6.90407966896291
H	-4.01801943786833	-0.97798924959210	-5.21820742035918
H	-4.43282118566353	-0.53313678112581	-6.88115341321378
H	-5.22729612054258	0.28396617502255	-5.53602958956812
H	-2.98805835865056	0.97255308591310	-3.64165611022966
H	-4.27847552971449	2.00499794421716	-4.31180035607936
H	-2.57991811177745	2.50967649002815	-4.39893612473071

H	-2.75171164012405	2.80939352157904	-6.91621620830456
H	-4.48186728654721	2.47047330744962	-6.70291313977764
H	-3.53983724997265	1.56915864909146	-7.91276911265319
H	2.90444330392614	-0.78766235148561	-5.02783130065630
H	4.10613022031950	0.43089293996535	-5.50001333879806
H	3.29940829540655	-0.53369587896712	-6.74357585436283
H	1.39959334842728	2.62654551131839	-4.43794496424433
H	3.08390461444929	2.09588699594612	-4.25770655209310
H	1.73822173924092	1.09192146454091	-3.64202502110352
C	0.84044442273604	-2.22970466045751	-9.55729519380124
C	-1.27492687947174	-1.13094256953275	-10.26092375884828
C	-1.32893671241217	-3.09989953190258	-8.71558983844263
H	-0.84066512423228	-3.62995326519597	-7.88497025377700
H	-1.37950797730186	-3.79077399510284	-9.57059623462591
H	-2.36134695381146	-2.88298760224402	-8.40736883996308
H	1.42956958861038	-1.36671930025040	-9.89990896735602
H	0.77261443665802	-2.92958803631636	-10.40235320655337
H	1.40900477324715	-2.73226155813293	-8.76129422162166
H	-0.75148210214957	-0.21105063630149	-10.55954242359098
H	-2.30919803794437	-0.85701707817050	-10.00937365611663
H	-1.31620463851793	-1.79280680531410	-11.13916348301560
H	1.62011047068712	2.85772566843431	-6.96755337571810
H	2.47838759233138	1.61186252499135	-7.89678068837322
H	3.34671904883073	2.56372813171961	-6.67262540223178

[Co](H$_2$)$^{1-}$

Co	0.02568489878249	0.07675865186360	-1.09214624742551
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P	1.65753492225358	-1.30770672325302	-0.85351659399440
P	-2.01129720965748	-0.62663300095154	-0.88005286984326
C	-0.52239078213721	1.32531375581129	1.76172127004348
C	-1.13074376915045	1.45628507237047	3.02128685315879
H	-1.27191340421058	0.56117643824226	3.63993202848083
C	-1.61453081459656	2.67966412205651	3.48593673937813
H	-2.10893465626280	2.73965696397791	4.46129589166230
C	-1.49502868273498	3.82295011882595	2.69686502982115
H	-1.89899913086663	4.77959166131387	3.04182550816886
C	-0.86525504769712	3.73215361027847	1.45415984585090
H	-0.78951568795089	4.62846365302335	0.82896266507018
C	-0.38109935378340	2.50123863198797	0.99584829974325
C	1.47003230703410	-0.44560784001106	1.68238151166611
C	1.92013697964641	-0.16400136348907	2.98297197715595
H	1.23174494569204	0.30947655093507	3.69416669199115
C	3.23313306732822	-0.41592819749476	3.38199660800837
H	3.55739561797736	-0.15946958833970	4.39612035000384

C	4.14296307161113	-0.96979780225120	2.48196833399089
H	5.18146165028049	-1.14331275378228	2.77991191850048
C	3.71837892404341	-1.28911464275029	1.19101420108496
H	4.43998697600803	-1.70585121707746	0.47975584529085
C	2.39885949290710	-1.03455777571132	0.79926177330180
C	-1.06861819055549	-1.26931375615172	1.55841630243373
C	-1.00478773069206	-1.98449265115600	2.76587837304471
H	-0.21418756957077	-1.74249301764631	3.48719398375022
C	-1.88074879067529	-3.03220369261599	3.05211752520810
H	-1.78408374452935	-3.58754610182698	3.99110772749707
C	-2.86371651511557	-3.39178497557324	2.13114812725921
H	-3.53561441083309	-4.23070998187706	2.33645983883374
C	-2.97378237043964	-2.67797598734428	0.93597351578422
H	-3.73471148005952	-2.97584065396629	0.20637120244582
C	-2.09110252564357	-1.62841256559076	0.65562065884803
C	-0.35020231917440	3.44361186091820	-1.78003512953374
H	-0.30196388213008	4.41882078512577	-1.26566619142035
C	-1.80739476041591	3.13839546574623	-2.06558260424073
H	-2.25792527858259	3.91225629694797	-2.70987278435482
H	-2.40136534884562	3.08395906584641	-1.14150383370194
H	-1.90799372766389	2.16750346389560	-2.57767916759258
C	0.44351844192178	3.53448444645935	-3.07349899256328
H	0.46652153585527	2.55751773898995	-3.58601993655813
H	1.48844329994607	3.84111242793316	-2.91748338411429
H	-0.01007867231597	4.25601181708700	-3.77325589106141
C	2.09569136685011	3.03550575940750	-0.36131344134286
H	2.66218073735288	2.80577427690190	-1.28167634075523
C	2.03948809583011	4.54866021241017	-0.19988876884968
H	1.43468468938032	4.83708041591908	0.67430571800477
H	1.64250556146885	5.08082220237243	-1.07541521840936
H	3.05313080421993	4.94670818834577	-0.02125686491943
C	2.85099860565046	2.44271228146150	0.81476844424998
H	3.83736854939372	2.92382164994582	0.92670572042953
H	3.01654423962018	1.36538936884208	0.71077461388457
H	2.30502133967807	2.59199418397139	1.76059740094115
C	3.11944208582973	-1.13016973629979	-2.04654909583254
H	3.95286701656180	-1.73850337827175	-1.65389200596011
C	2.74123730142016	-1.64994147576449	-3.42495542513337
H	1.88019292263516	-1.09214758315285	-3.82918971722778
H	2.46358397488290	-2.71457673536366	-3.42212391329585
H	3.57052678586635	-1.52951154439768	-4.14192004051568
C	3.58852150076703	0.30951278718332	-2.12708653871389
H	4.45561336129333	0.40964670653196	-2.80167420780080
H	3.88472618469816	0.69889255291412	-1.14195704439759
H	2.78394537712839	0.95932458468945	-2.50800182826659
C	1.57114258954265	-3.22667695146270	-0.87168881595221

H	1.05218556342286	-3.45988531290434	-1.81912993761181
C	2.90708901362963	-3.95683363716244	-0.86446829874032
H	3.49945987980076	-3.70199612185743	0.02872681720918
H	3.52947441365503	-3.76122047021590	-1.74878821036139
H	2.74302938101819	-5.04751127135910	-0.82806623890429
C	0.71364549193536	-3.74505333853085	0.26889032596275
H	0.62099026396464	-4.84322099348793	0.22027237540043
H	-0.29743782483559	-3.32424598406113	0.25877122857228
H	1.15266989474511	-3.49649206866702	1.24895858551386
C	-2.63882464702224	-1.81879609444951	-2.21314078979774
H	-3.57979353316766	-2.26337772521575	-1.84576723821549
C	-2.92667947044345	-1.05995045917911	-3.49924579220052
H	-2.01579052547269	-0.56052257135510	-3.86924688287309
H	-3.69338645094939	-0.28053873578581	-3.37485256136070
H	-3.27329438487320	-1.73693196408533	-4.29794267081137
C	-1.66182911962460	-2.95132418035788	-2.46388097514032
H	-2.06021253793580	-3.66057699590981	-3.20904443750668
H	-1.44551870449739	-3.51743942234114	-1.54597425155870
H	-0.70210470629497	-2.56613020171114	-2.84497409203627
C	-3.63723533264582	0.39084258314558	-0.70155475694828
H	-3.60756491146573	1.08450190526029	-1.56129095769557
C	-4.94089443999368	-0.39298898541097	-0.76886669208420
H	-4.99699971834190	-1.15205624621686	0.02736710726209
H	-5.11221393282127	-0.89774373209863	-1.72987105144627
H	-5.79753789253212	0.28498516633633	-0.61192146132799
C	-3.62515672069461	1.22092568547672	0.57003390792665
H	-4.53631889537962	1.83882977165614	0.64142110805122
H	-2.76284951495108	1.89366656160029	0.62778653456341
H	-3.59210332541889	0.58216022469706	1.46782444938500
H	0.09844247936659	0.57335909315864	-2.63649331281483
H	0.00867678722319	-0.30996418175742	-2.65777123452086

[Co](H)$_2$$^{1-}$

Co	0.01729694158858	0.10184206322372	-1.16915089209566
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P	1.67557837984134	-1.29279952277422	-0.90099304011551
P	-1.99263783978642	-0.66793489921197	-0.96813604118823
C	-0.41458077271509	1.42882509102401	1.92728774767901
C	-0.90157699893789	1.69933210044427	3.21436400304101
H	-0.95275445366707	0.87965221454052	3.94162722100577
C	-1.37487460796969	2.95593686107938	3.59124491439390
H	-1.76430439296603	3.11863656005412	4.60111909329341
C	-1.37470533133860	3.99325224536779	2.66346635904833
H	-1.76612866111231	4.97919981459456	2.93133051954545
C	-0.87344701584326	3.76475049586077	1.38136060547871

H	-0.88964528516211	4.58904398000812	0.66154206143092
C	-0.38335335796780	2.50788361923149	0.99836584174485
C	1.46336573615726	-0.59857765987436	1.85426467994561
C	1.97620560950673	-0.49453955219933	3.15450187095277
H	1.32799300454533	-0.10153937467320	3.94752204976981
C	3.29538778883783	-0.82141989507165	3.46888963427154
H	3.66208429490511	-0.71053463516695	4.49421596975976
C	4.14959440462999	-1.26130014463233	2.46192208682238
H	5.19484805944418	-1.49693483135812	2.68335176638823
C	3.66400629402341	-1.39485529203493	1.16055635882536
H	4.35338440770500	-1.72904038571812	0.37908956352520
C	2.33502628657040	-1.08315820813628	0.83923197942975
C	-1.18683122619414	-1.18107425108417	1.66612042730265
C	-1.29205421624653	-1.83983848690932	2.90174131155076
H	-0.61210817671097	-1.55356356730822	3.71316813532759
C	-2.18602083097343	-2.88688462905150	3.12359645196325
H	-2.21731905880674	-3.38697757659395	4.09665688039808
C	-3.01349949936833	-3.31318229451093	2.08862741334905
H	-3.69851490532799	-4.15392891990798	2.23370237031268
C	-2.95863627328990	-2.65756120616199	0.85871979163079
H	-3.60886412161405	-3.00459342976530	0.04963892743458
C	-2.07349910525338	-1.59248763397263	0.63779166439207
C	-0.50234160176880	3.51036171742279	-1.80606389922837
H	-0.42054039457447	4.49898458211845	-1.32186664193781
C	-1.96988946340231	3.19770295683624	-2.02263036460753
H	-2.44985352225984	3.96053776785526	-2.65828989740695
H	-2.52647375181538	3.15259162142863	-1.07427915752644
H	-2.07868309455239	2.22044206387882	-2.51939305287668
C	0.24100312006384	3.55072060392273	-3.13433943600279
H	0.24083723126589	2.55140154886859	-3.59974392556112
H	1.29149197708349	3.86027214805799	-3.02588045193149
H	-0.23731008944894	4.25233623066709	-3.83761128054917
C	1.99935097740607	3.08701509048113	-0.44984768853001
H	2.56115699414607	2.84722117499731	-1.36965625948128
C	1.97208131159628	4.59918610357010	-0.28844680722555
H	1.37220600324789	4.90183660962931	0.58456908863813
H	1.58162862160716	5.13154997123993	-1.16765905100737
H	2.99250783185340	4.98191689950365	-0.11367149786354
C	2.73024052775986	2.45985680315058	0.72444865443506
H	3.77808347634407	2.80079921215897	0.76898817318950
H	2.73776580248761	1.36409977653721	0.67113582009566
H	2.25583940679842	2.72883435198495	1.68215493516453
C	3.18312060650391	-1.09769540411467	-2.01636027884936
H	3.99874135923262	-1.74297717845456	-1.64665732024308
C	2.79692786886485	-1.54468747041578	-3.41971896890212
H	1.93924569071568	-0.95376389193356	-3.78119069690659

H	2.50486042115568	-2.60479080095074	-3.46655375720687
H	3.63018932094660	-1.40180215997430	-4.12759740824716
C	3.67206057370542	0.33696027514815	-2.03107762126399
H	4.53936484457619	0.45413585109401	-2.70231628905688
H	3.97443114274719	0.68145859079440	-1.03083956013813
H	2.87014137911965	1.00420491919115	-2.38571335816227
C	1.58792651125517	-3.21543344340956	-0.91220405895898
H	1.04848483620828	-3.43995860937286	-1.84841512008116
C	2.90733715535537	-3.97283575914142	-0.93793127120427
H	3.51860668224907	-3.75646331666657	-0.04767466301381
H	3.51996277065937	-3.76933315304435	-1.82757414631123
H	2.71746953691423	-5.06013517268136	-0.92669606793537
C	0.74349552688849	-3.71289087138428	0.24819873237527
H	0.52847732450300	-4.79009742649913	0.14769804763327
H	-0.21546310964991	-3.18717299909543	0.32348184695206
H	1.26117617928052	-3.57006777010113	1.21078412401239
C	-2.59146960746119	-1.89456111231876	-2.26547028689426
H	-3.52847751859614	-2.36222775894764	-1.91613542340770
C	-2.86810774665920	-1.14153421454051	-3.55926622708835
H	-1.95704422528546	-0.61970713251090	-3.89468003741320
H	-3.65821845223070	-0.38283374589861	-3.45262367127103
H	-3.17954102245541	-1.82938620472800	-4.36291213883517
C	-1.56449086583988	-2.98609642223056	-2.49256147251629
H	-1.91122911206003	-3.70825994945751	-3.25084956211508
H	-1.34882456121817	-3.54592430342375	-1.56997182323262
H	-0.61791637972625	-2.54503666225068	-2.84399635282674
C	-3.62818075838323	0.32697675620464	-0.76993353621285
H	-3.60486198880907	1.03671958726529	-1.61472782417115
C	-4.92714485224908	-0.46123526861849	-0.85221734900803
H	-4.98718700860450	-1.22746566915733	-0.06317748755550
H	-5.08510949456437	-0.95871788226583	-1.81953439869165
H	-5.78832019468148	0.21178868992975	-0.69796136874092
C	-3.60721313422990	1.12953722717104	0.51952200923244
H	-4.45060989702404	1.83950166181145	0.55744296538698
H	-2.68183044143794	1.70477360952032	0.64039625943461
H	-3.69124714480440	0.47376084820759	1.40153708343006
H	0.27684999159377	0.18564246863132	0.32136663690603
H	0.02797624625903	0.17959147528975	-2.68777509205924

TS $[Co](H_2)^{1-} \rightarrow [Co](H)_2^{1-}$

Co	-0.197386	-0.061320	-1.182320
B	0.060024	-0.116773	1.165808
P	-0.160735	2.140574	-0.738975
P	1.775108	-0.953840	-0.955096
P	-2.138326	-0.980030	-0.588746
C	-0.591749	1.240933	1.776009

C	-1.041110	1.323323	3.106986
H	-0.981304	0.434216	3.745695
C	-1.603252	2.484379	3.631842
H	-1.955932	2.503213	4.668350
C	-1.737431	3.617180	2.829900
H	-2.197771	4.527548	3.225033
C	-1.292915	3.571531	1.509618
H	-1.425965	4.457566	0.881490
C	-0.725787	2.400368	0.987551
C	1.627963	-0.150368	1.585894
C	2.105713	0.215921	2.856845
H	1.393883	0.543683	3.623532
C	3.465841	0.221036	3.161782
C	4.400665	-0.152157	2.195661
H	5.470503	-0.134668	2.424125
C	3.957750	-0.535786	0.930520
H	4.693950	-0.819790	0.171188
C	2.589995	-0.526713	0.631973
C	-0.775590	-1.361589	1.750961
C	-0.484686	-1.981104	2.979452
H	0.392421	-1.648202	3.547911
C	-1.254320	-3.027869	3.481730
H	-0.987142	-3.500363	4.432882
C	-2.361003	-3.480778	2.764993
H	-2.964511	-4.312297	3.140836
C	-2.683084	-2.873120	1.550901
H	-3.538624	-3.257949	0.987824
C	-1.899502	-1.828232	1.042987
C	-1.299291	3.320988	-1.677835
H	-1.307441	4.258079	-1.097427
C	-2.718889	2.800053	-1.744873
H	-3.386905	3.537734	-2.220414
H	-3.126832	2.575963	-0.750007
H	-2.753966	1.882934	-2.353006
C	-0.780938	3.611468	-3.070597
H	-0.738090	2.687907	-3.663419
H	0.225174	4.054112	-3.086015
H	-1.449004	4.308077	-3.606041
C	1.393421	3.256404	-0.759034
H	1.798208	3.124887	-1.779108
C	1.145983	4.740996	-0.518298
H	0.710147	4.914785	0.478036
H	0.500611	5.228191	-1.260259
H	2.107833	5.279979	-0.532541
C	2.435489	2.789030	0.241132
H	3.336934	3.421410	0.183326

H	2.747145	1.753600	0.083076
H	2.056976	2.852399	1.274274
C	3.107464	-0.649843	-2.272095
H	4.085726	-0.832480	-1.792230
C	2.969631	-1.600604	-3.452173
H	1.928800	-1.720894	-3.785190
H	3.342928	-2.609833	-3.231047
H	3.540538	-1.231054	-4.320361
C	3.058193	0.790422	-2.741034
H	3.810685	0.977690	-3.525014
H	3.243671	1.499288	-1.923181
H	2.059977	0.999621	-3.160035
C	1.963771	-2.843870	-0.871520
H	1.597106	-3.188358	-1.856917
C	3.394213	-3.329737	-0.666693
H	3.743003	-3.089996	0.349597
H	4.131345	-2.919090	-1.369359
H	3.434468	-4.427527	-0.760825
C	1.098137	-3.461369	0.206724
H	1.164754	-4.561831	0.179684
H	0.046930	-3.181772	0.106825
H	1.423391	-3.136328	1.207502
C	-2.798391	-2.454037	-1.581597
H	-3.624603	-2.830181	-0.958461
C	-3.398392	-2.094646	-2.930253
H	-2.645371	-1.882135	-3.701725
H	-4.073952	-1.225543	-2.910601
H	-3.993865	-2.944550	-3.306216
C	-1.809026	-3.600382	-1.723449
H	-2.175790	-4.337146	-2.456626
H	-1.645293	-4.125769	-0.772185
H	-0.828679	-3.243218	-2.071594
C	-3.851261	-0.140862	-0.285637
H	-3.967219	0.513272	-1.167321
C	-5.081627	-1.036992	-0.212997
H	-5.018074	-1.751660	0.622304
H	-5.287649	-1.602149	-1.131660
H	-5.972973	-0.416904	-0.018029
C	-3.826973	0.727314	0.961292
H	-4.779411	1.272136	1.074120
H	-3.022528	1.467710	0.957194
H	-3.689109	0.115652	1.867795
H	-0.218898	0.196236	-2.750778
H	-0.277590	-1.438376	-1.732352
B	-0.817872	0.502606	-5.270763
C	0.010087	-0.816590	-5.538686

C	-2.361132	0.498721	-4.899185
C	-0.166116	1.813814	-5.895062
C	1.301043	2.149308	-5.682098
H	-0.773036	2.714681	-5.714916
H	-0.332359	1.614483	-6.976833
H	3.803484	0.532530	4.155812
H	-2.816110	-0.412470	-5.328750
C	-3.185150	1.717579	-5.284666
H	-2.453716	0.328576	-3.807453
C	-0.358148	-2.180580	-4.992314
H	1.075879	-0.615772	-5.336758
H	-0.013046	-0.868516	-6.649909
H	1.477573	2.579812	-4.682634
H	1.666437	2.894881	-6.406420
H	1.963817	1.274639	-5.762503
H	-3.110989	1.957107	-6.357862
H	-2.857494	2.612717	-4.734002
H	-4.255893	1.589447	-5.057826
H	-0.274588	-2.235765	-3.895345
H	0.294535	-2.972926	-5.395163
H	-1.389158	-2.484215	-5.235308

BEt_3

B	0.57684642386477	0.20679594936310	0.15683853152277
C	2.07434328592726	0.61453889767454	-0.10166093393962
C	-0.03334215328976	0.33086660197166	1.60164286025525
C	-0.30921002346714	-0.32619907882650	-1.02889085722364
C	0.84422556580204	0.84149432293684	2.73007338408682
H	-0.94721044456452	0.95026895222013	1.51194678353010
H	-0.45718914921450	-0.65933400451819	1.85990934967171
H	2.69115539048316	0.03302225676539	0.61146361154758
H	2.20065968990902	1.64648182273419	0.27998386724778
C	2.63691491146112	0.49649976643266	-1.50660579116550
H	0.23936419216643	-1.17365524684481	-1.48466708843461
H	-0.26072555683597	0.43315764689597	-1.83378131425780
C	-1.75028474533209	-0.71555267396722	-0.75335228501190
H	2.58292562090894	-0.53547685635403	-1.88492673022639
H	3.69107020796638	0.80290360085304	-1.57163039314465
H	2.08130661145778	1.11897638226732	-2.22416981477745
H	-1.82181294639003	-1.52082417551227	-0.00674172619166
H	-2.27615451984578	-1.06953299741078	-1.65196568643487
H	-2.33451783966876	0.12814186633544	-0.35598123606336
H	1.72870847579674	0.20442251763038	2.88188345350669
H	0.31754854494875	0.88614192098602	3.69433711217921
H	1.22335845791615	1.85472252836713	2.52861490332353

$HBEt_3$

B	0.66772506925702	-0.08973280109216	0.21894455047309
C	1.99826654307583	0.79042567521066	-0.18345788997764
C	-0.04874382846695	0.52948935805414	1.56428576043682
C	-0.39736676068933	-0.13195473096726	-1.03420896115204
C	0.85533526444539	0.68297372726015	2.77673529791713
H	-0.49557838168366	1.52245052484351	1.33073582341865
H	-0.91505469792482	-0.09764496190700	1.85900807162346
H	2.73385864262769	0.77254465931992	0.64674132689529
H	1.72409148768162	1.86507176817179	-0.28400951070887
C	2.71187714253591	0.35588552008674	-1.45348526776148
H	0.07748624717731	-0.59381275489750	-1.92407678825931
H	-0.63898751291653	0.90537715024324	-1.35944712611691
C	-1.70039758331750	-0.86611741167960	-0.76193792022300
H	2.97924895647073	-0.71516501750183	-1.41072745363210
H	3.64661724408687	0.90967279096088	-1.67227014064580
H	2.06903999829780	0.46994395383054	-2.34359176424271
H	-1.50852396462676	-1.89494355515031	-0.40816834966481
H	-2.37641546077175	-0.95019213301005	-1.63614553838853
H	-2.28613806674632	-0.37800879937517	0.03631084670537
H	1.34493990198151	-0.27458180566989	3.02937767714318
H	0.34303810312775	1.03169387895213	3.69556661555187
H	1.67420992765804	1.39888732577943	2.58848860562098
H	1.03399172872013	-1.27376236146236	0.47111213498735

TS $[Co](H_2)^{1-} \rightarrow [Co](H)$

Co	-0.197386	-0.061320	-1.182320
B	0.060024	-0.116773	1.165808
P	-0.160735	2.140574	-0.738975
P	1.775108	-0.953840	-0.955096
P	-2.138326	-0.980030	-0.588746
C	-0.591749	1.240933	1.776009
C	-1.041110	1.323323	3.106986
H	-0.981304	0.434216	3.745695
C	-1.603252	2.484379	3.631842
H	-1.955932	2.503213	4.668350
C	-1.737431	3.617180	2.829900
H	-2.197771	4.527548	3.225033
C	-1.292915	3.571531	1.509618
H	-1.425965	4.457566	0.881490
C	-0.725787	2.400368	0.987551
C	1.627963	-0.150368	1.585894
C	2.105713	0.215921	2.856845
H	1.393883	0.543683	3.623532
C	3.465841	0.221036	3.161782
C	4.400665	-0.152157	2.195661

H	5.470503	-0.134668	2.424125
C	3.957750	-0.535786	0.930520
H	4.693950	-0.819790	0.171188
C	2.589995	-0.526713	0.631973
C	-0.775590	-1.361589	1.750961
C	-0.484686	-1.981104	2.979452
H	0.392421	-1.648202	3.547911
C	-1.254320	-3.027869	3.481730
H	-0.987142	-3.500363	4.432882
C	-2.361003	-3.480778	2.764993
H	-2.964511	-4.312297	3.140836
C	-2.683084	-2.873120	1.550901
H	-3.538624	-3.257949	0.987824
C	-1.899502	-1.828232	1.042987
C	-1.299291	3.320988	-1.677835
H	-1.307441	4.258079	-1.097427
C	-2.718889	2.800053	-1.744873
H	-3.386905	3.537734	-2.220414
H	-3.126832	2.575963	-0.750007
H	-2.753966	1.882934	-2.353006
C	-0.780938	3.611468	-3.070597
H	-0.738090	2.687907	-3.663419
H	0.225174	4.054112	-3.086015
H	-1.449004	4.308077	-3.606041
C	1.393421	3.256404	-0.759034
H	1.798208	3.124887	-1.779108
C	1.145983	4.740996	-0.518298
H	0.710147	4.914785	0.478036
H	0.500611	5.228191	-1.260259
H	2.107833	5.279979	-0.532541
C	2.435489	2.789030	0.241132
H	3.336934	3.421410	0.183326
H	2.747145	1.753600	0.083076
H	2.056976	2.852399	1.274274
C	3.107464	-0.649843	-2.272095
H	4.085726	-0.832480	-1.792230
C	2.969631	-1.600604	-3.452173
H	1.928800	-1.720894	-3.785190
H	3.342928	-2.609833	-3.231047
H	3.540538	-1.231054	-4.320361
C	3.058193	0.790422	-2.741034
H	3.810685	0.977690	-3.525014
H	3.243671	1.499288	-1.923181
H	2.059977	0.999621	-3.160035
C	1.963771	-2.843870	-0.871520
H	1.597106	-3.188358	-1.856917

C	3.394213	-3.329737	-0.666693
H	3.743003	-3.089996	0.349597
H	4.131345	-2.919090	-1.369359
H	3.434468	-4.427527	-0.760825
C	1.098137	-3.461369	0.206724
H	1.164754	-4.561831	0.179684
H	0.046930	-3.181772	0.106825
H	1.423391	-3.136328	1.207502
C	-2.798391	-2.454037	-1.581597
H	-3.624603	-2.830181	-0.958461
C	-3.398392	-2.094646	-2.930253
H	-2.645371	-1.882135	-3.701725
H	-4.073952	-1.225543	-2.910601
H	-3.993865	-2.944550	-3.306216
C	-1.809026	-3.600382	-1.723449
H	-2.175790	-4.337146	-2.456626
H	-1.645293	-4.125769	-0.772185
H	-0.828679	-3.243218	-2.071594
C	-3.851261	-0.140862	-0.285637
H	-3.967219	0.513272	-1.167321
C	-5.081627	-1.036992	-0.212997
H	-5.018074	-1.751660	0.622304
H	-5.287649	-1.602149	-1.131660
H	-5.972973	-0.416904	-0.018029
C	-3.826973	0.727314	0.961292
H	-4.779411	1.272136	1.074120
H	-3.022528	1.467710	0.957194
H	-3.689109	0.115652	1.867795
H	-0.218898	0.196236	-2.750778
H	-0.277590	-1.438376	-1.732352
B	-0.817872	0.502606	-5.270763
C	0.010087	-0.816590	-5.538686
C	-2.361132	0.498721	-4.899185
C	-0.166116	1.813814	-5.895062
C	1.301043	2.149308	-5.682098
H	-0.773036	2.714681	-5.714916
H	-0.332359	1.614483	-6.976833
H	3.803484	0.532530	4.155812
H	-2.816110	-0.412470	-5.328750
C	-3.185150	1.717579	-5.284666
H	-2.453716	0.328576	-3.807453
C	-0.358148	-2.180580	-4.992314
H	1.075879	-0.615772	-5.336758
H	-0.013046	-0.868516	-6.649909
H	1.477573	2.579812	-4.682634
H	1.666437	2.894881	-6.406420

H	1.963817	1.274639	-5.762503
H	-3.110989	1.957107	-6.357862
H	-2.857494	2.612717	-4.734002
H	-4.255893	1.589447	-5.057826
H	-0.274588	-2.235765	-3.895345
H	0.294535	-2.972926	-5.395163
H	-1.389158	-2.484215	-5.235308

TS $[Co](H)_2^{1-} \rightarrow [Co](H)$

Co	0.04146466101606	0.09034905751118	-1.33037556423591
B	-0.05012235344375	-0.11350168788927	1.42390538005289
P	0.27156511566602	2.26938755079636	-0.71904716565623
P	1.82448914701609	-1.29194857017756	-0.88152501171763
P	-1.99638080491562	-0.81618586973827	-1.03508552196937
C	-0.41154314907284	1.37817049026881	1.90313774709722
C	-0.88306826720569	1.59765162725351	3.20738167250854
H	-1.02675875881312	0.73633851019485	3.86975399776052
C	-1.21316288498160	2.86461423932971	3.68051571622346
H	-1.58731422948115	2.99230649647264	4.70070970171247
C	-1.07984142454865	3.96283651111239	2.83625875514954
H	-1.34230020483690	4.96676876188714	3.18184099939308
C	-0.62429356238554	3.77252801837990	1.53347479127637
H	-0.55500928226673	4.64698017667213	0.88209450277990
C	-0.29058432115290	2.49797755337976	1.04737247663614
C	1.42234393031165	-0.60142826150435	1.84896758816179
C	1.85024581019659	-0.47798467879775	3.18001549883896
H	1.16665382586253	-0.04336356399587	3.91825622188232
C	3.12892459632966	-0.84566776454925	3.59072023838454
H	3.42788795248841	-0.72601426393549	4.63639981612385
C	4.02867429757663	-1.34314363645685	2.65290925010109
H	5.04388119505740	-1.62224907113103	2.94906582895508
C	3.63186542916169	-1.47097439498747	1.32314423615768
H	4.36423954962279	-1.84233164419051	0.60253106574571
C	2.34139219340705	-1.11075063379080	0.90270436892910
C	-1.21495949061831	-1.18600335075687	1.66086306876066
C	-1.32921308416169	-1.79587841654721	2.92133754727007
H	-0.59616958403725	-1.54936406911072	3.69786712140371
C	-2.31371291829783	-2.73654564928994	3.21084846711339
H	-2.36231776217173	-3.19605928957863	4.20261534129424
C	-3.22017020091832	-3.10278329207359	2.21990087905435
H	-3.99243472903090	-3.85099731510421	2.42010655345661
C	-3.12525502719214	-2.51914245692025	0.95859066863750
H	-3.82797617252776	-2.84199470107055	0.18659456962952
C	-2.13852016025887	-1.56506817438355	0.66194321638217
C	-0.59810797109974	3.71509225140994	-1.55143277168356
H	-0.26986147301163	4.63577919232330	-1.04352722776773

C	-2.10958363140175	3.63598785724579	-1.46868365471737
H	-2.57172159548737	4.42757580003581	-2.08090026106069
H	-2.48310590395277	3.74551892810198	-0.44104961699432
H	-2.47203990262747	2.67341939279455	-1.85777195069859
C	-0.14614713993387	3.75163135892163	-2.99337478547675
H	-0.43968783517929	2.81358876194981	-3.47745593931583
H	0.94387717665030	3.85249881534773	-3.10959808670741
H	-0.62457506713251	4.57767780995120	-3.54503292722113
C	2.02088631906495	3.04046080668309	-0.57766125389442
H	2.48558097106501	2.75760011468894	-1.53886461447644
C	2.13187741499583	4.55063945965267	-0.43466747715236
H	1.61492653114674	4.91714169537609	0.46652240709476
H	1.74745137987991	5.10632974930787	-1.30072901510682
H	3.19155678870350	4.83445535093129	-0.32124571118147
C	2.78338457432496	2.36601654706238	0.54888291077588
H	3.85615471679739	2.61531947292288	0.50819211063622
H	2.69583340304454	1.27341271111563	0.51348486749383
H	2.40468651899900	2.68666261881942	1.53261241559212
C	3.48058581688647	-1.16381950478194	-1.76339626049542
H	4.15679051341469	-1.92028713505297	-1.33360916147751
C	3.23605700801457	-1.49968872513352	-3.21924918608633
H	2.45566424375552	-0.84743608100224	-3.62861356359455
H	2.88723299601038	-2.53415351918355	-3.36120853443651
H	4.14312089861610	-1.36769101524118	-3.83151583080462
C	4.11852718055291	0.19981464172388	-1.59244235552635
H	4.96665463537281	0.32680419648995	-2.28464048055668
H	4.49040843396417	0.35913360720104	-0.57022533554237
H	3.39320550586038	0.99683521729661	-1.80887735998097
C	1.64881605370658	-3.20119331547241	-0.90940757874178
H	1.13949175310534	-3.39023109873176	-1.87136199145384
C	2.92688596564685	-4.02634852359427	-0.88221757728796
H	3.52196409801663	-3.82565232590879	0.02290789733280
H	3.57382720591710	-3.87802982765615	-1.75725955793688
H	2.67299134315506	-5.09922850643008	-0.85409801041868
C	0.74173656765110	-3.65230117369427	0.22165456560961
H	0.44760587297445	-4.70696961077869	0.09542264020600
H	-0.17632967769796	-3.05749235820481	0.28386491379303
H	1.24849928083058	-3.56388149015197	1.19624666984204
C	-2.69090317555581	-2.20882881269929	-2.09534871571556
H	-3.71295266503615	-2.42461813482932	-1.74487101799714
C	-2.74456493811415	-1.71055814157756	-3.52139545974992
H	-1.73455161875298	-1.41276510589379	-3.82506490119611
H	-3.39527588468972	-0.83258330431694	-3.65478001700086
H	-3.09002902786946	-2.49730755873511	-4.21208568191132
C	-1.87611709948460	-3.48349117822766	-2.00527538301733
H	-2.21500509192618	-4.21581772068689	-2.75627711552669

H	-1.94463900550619	-3.96005302101225	-1.01753487254335
H	-0.81563129294070	-3.27767621103480	-2.20809378149192
C	-3.55053420667862	0.30172537403208	-0.99531514580820
H	-3.38864703284239	0.96989381215644	-1.86050921913488
C	-4.91189054194844	-0.35417640105951	-1.16746480242681
H	-5.11660885407011	-1.09045530715388	-0.37435075459109
H	-5.04351707460723	-0.85080796432109	-2.13863650462613
H	-5.70349524840984	0.41011134074139	-1.09280824803953
C	-3.54432886648476	1.13289526092937	0.27590662658494
H	-4.27783742324119	1.95344773873878	0.21827960533628
H	-2.56270197863415	1.57863098684403	0.47884165738932
H	-3.80319763972604	0.51689238403342	1.15215960559489
H	0.14742683672690	0.07824968693035	0.19891964161995
H	0.09056517036955	0.22306167553502	-3.22641158717737
B	0.14724060425765	0.38039332099340	-4.93497948649194
C	-1.36363101173801	0.59680000473937	-5.47669882985189
C	0.79336378388209	-0.98428113353632	-5.52621486320941
C	1.10561929124153	1.64280341365815	-5.26550301649382
C	0.27757863234913	-2.34521927699775	-5.09613361278692
H	1.89143511221103	-0.97835476758796	-5.43123496786711
H	0.63176370499168	-0.88378892345985	-6.61882501687306
H	-1.93830977256275	-0.34200913542317	-5.48223699097858
H	-1.20063946765255	0.80853427259052	-6.55340583960053
C	-2.24323850447305	1.69236049870615	-4.90568861613248
H	0.61115106705458	2.61490165060448	-5.12075230611063
H	1.23490422284608	1.57573299521952	-6.36539794882977
C	2.48249840001692	1.71463771475119	-4.63106580848081
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H	3.04887890828242	2.62110880503631	-4.90932803682042
H	3.11636279703972	0.85736031667628	-4.90924744488193
H	0.31751150270472	-2.46544182137246	-3.99890331841739
H	0.85519924848245	-3.18324088507546	-5.52535260125287
H	-0.76982369292950	-2.50587472555127	-5.40091034157216
H	-2.37081673667952	1.58229258229254	-3.81438627692777
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B	-0.00457459748165	-0.19693572510115	1.27620481495340
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P	1.89955962171358	-1.23855092346848	-0.86213685897544
P	-2.18504185806898	-0.58798642847325	-0.79286694004321
C	-0.51665616258608	1.27636089885612	1.77390007676631
C	-1.10070717146973	1.44678037866617	3.05474236923244
H	-1.22749198946701	0.56762058924620	3.70798759512382

C	-1.56489436705579	2.69466803691388	3.50494767233929
H	-2.02042013616061	2.78345266293517	4.50461675449841
C	-1.47458599113624	3.82349253548337	2.67262639348100
H	-1.85866927326496	4.79913936588245	3.01000091634404
C	-0.89894626640055	3.69350141305163	1.39735627114011
H	-0.84754519905435	4.57462752140909	0.73820040458759
C	-0.41965411614724	2.43998252297683	0.95850241604763
C	1.52077682914987	-0.53729181717694	1.75824593812324
C	1.93349270289290	-0.33609745484099	3.09981936614039
H	1.21585596169834	0.07743724967209	3.82708636372460
C	3.24387225035474	-0.60827073569580	3.52942463807252
H	3.52559745105699	-0.42834931417562	4.57964687727922
C	4.20096316565757	-1.08984560367437	2.61984243174026
H	5.23302556294555	-1.29091820105174	2.94777942748034
C	3.83113348626100	-1.30016796268360	1.28128829072477
H	4.58578286388479	-1.65909329391906	0.56320155248385
C	2.51101990290229	-1.02847423415731	0.85968934139200
C	-1.10299095567835	-1.35086006572826	1.62411284635540
C	-1.03363343276256	-2.13434191339127	2.80298762982242
H	-0.18091633440937	-1.99836727799958	3.48846387118817
C	-2.00422684030307	-3.10253348029559	3.11519218124987
H	-1.91090262923617	-3.69615355114186	4.03925057919968
C	-3.08150898276600	-3.32786141211870	2.24236119906096
H	-3.83651746814523	-4.09651531053991	2.47127143898046
C	-3.17957854501522	-2.57242381319033	1.06060422927994
H	-4.00964332870703	-2.77258757689709	0.36482060574578
C	-2.20922291248588	-1.59399550234918	0.75787780862466
C	-0.39228966901000	3.28226857088407	-1.95668592262428
H	-0.25923975491478	4.31227841401910	-1.56478805760491
C	-1.88919954733855	3.05148034768898	-2.17031609372191
H	-2.29323350195194	3.80227770801634	-2.88332486621495
H	-2.46066371743351	3.13970410706265	-1.22610004131476
H	-2.07940649183666	2.04633824415547	-2.59719553105311
C	0.37811381027034	3.15604901750047	-3.28352341201783
H	0.30548629982457	2.12371754066283	-3.68781735233474
H	1.45437980178218	3.40227584006688	-3.18372094780839
H	-0.04842490046147	3.84178050751270	-4.04678203915434
C	2.07035591169694	3.03102743445975	-0.42810067408232
H	2.65974242640006	2.71445515659499	-1.31307408045531
C	2.00874827142413	4.56844433632097	-0.42434013586524
H	1.38075585557009	4.95291900974106	0.40545709126061
H	1.64133195711572	5.00571024468321	-1.37327754825200
H	3.03220090107518	4.97035004003297	-0.26159696045284
C	2.79730401672798	2.54746312877172	0.83403434922274
H	3.81339988799343	2.99498640817106	0.87805493525501
H	2.90525301071771	1.44934029141086	0.87244911720608

H	2.25492638881091	2.85736556168615	1.75054437483398
C	3.35367270925531	-0.93325122966134	-2.05492798889392
H	4.13007773629854	-1.67255732059370	-1.76603866931180
C	2.89798685422255	-1.23094907015317	-3.49477073704138
H	2.08366251870786	-0.54016505171545	-3.80107468512772
H	2.52635855873963	-2.26664677923647	-3.62722067631376
H	3.74018647448654	-1.08719603984364	-4.20501134108274
C	3.97375304073149	0.46167094382862	-1.96009847382987
H	4.88802802684260	0.51233254752672	-2.58974643623767
H	4.25992379965728	0.73027784454312	-0.92484588005601
H	3.27246721708225	1.23164702994755	-2.33753914221806
C	1.76489974689956	-3.15058908254968	-1.03933230694928
H	1.18948000573429	-3.27101199095190	-1.98470441605796
C	3.09512833619717	-3.91114692051971	-1.17099166440026
H	3.74662687042444	-3.74736830806129	-0.28731131570631
H	3.67028688826082	-3.65351200441632	-2.08159914831192
H	2.89029488994089	-5.00216212225288	-1.21835453137297
C	0.93846468847496	-3.75567252195024	0.10374649426236
H	0.73539492476400	-4.82775379495209	-0.10389838951831
H	-0.03178470338982	-3.24520129397945	0.24384704191961
H	1.48556943449803	-3.69547091918649	1.06657728601651
C	-2.75782816525276	-1.74726783307186	-2.19594966072783
H	-3.79164637446122	-2.04427519174916	-1.92479796853879
C	-2.80574752559377	-0.96555283835099	-3.52063015884720
H	-1.79234996869694	-0.61382538087211	-3.81017064011151
H	-3.46858913395008	-0.07769829375176	-3.47236142655201
H	-3.17960894126853	-1.61245692400889	-4.34317399723288
C	-1.93834394504014	-3.03459400515966	-2.34147608449178
H	-2.42885728998983	-3.70853733623470	-3.07702003559274
H	-1.85178173920559	-3.58540628377929	-1.38445805762007
H	-0.91353324960445	-2.82852777152670	-2.71041584210624
C	-3.78475745396181	0.50010868994431	-0.63578488368156
H	-3.67928384583659	1.21743192499317	-1.47609798915268
C	-5.12847366953689	-0.23023511684521	-0.80771837383475
H	-5.28125578944122	-1.00687638131958	-0.03059423420838
H	-5.26017693751916	-0.69885288710726	-1.80255405505123
H	-5.95493231408896	0.50399296440263	-0.68916548373441
C	-3.79565518784454	1.29423950331206	0.67686439813432
H	-4.67360624178119	1.97537197848034	0.69688394755733
H	-2.88735225958312	1.90715685642392	0.81279731728561
H	-3.87578847554145	0.61931583275561	1.55338800039709
H	-0.31746500938540	-1.54342301766857	-1.05064784616460

[Co](H$_2$)H

Co	0.10303014918642	0.16159227090750	-1.09131574505075
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P	1.72974059036593	-1.38871992920596	-0.81515561323441
P	-1.98735579424955	-0.68116532558877	-0.95298297041389
C	-0.45333847328951	1.45879727823566	1.91114912672508
C	-0.91869766179744	1.66223517378246	3.23236109643766
H	-0.96257073710425	0.80485699226086	3.92371249823125
C	-1.37205161169283	2.91255741591167	3.68631768532371
H	-1.73703879761967	3.02317544612324	4.72009200662927
C	-1.37901067150047	4.01411233307207	2.81598356929561
H	-1.74645073193601	4.99489239295283	3.15651202611622
C	-0.92283002074322	3.85160153004150	1.49720546244915
H	-0.94683234561514	4.71605661768520	0.81507741544143
C	-0.46397015466472	2.59452013676520	1.04398768699316
C	1.51074306728171	-0.53469373050654	1.86864026239410
C	1.99819425097561	-0.36050225633566	3.18428977735700
H	1.36975879694148	0.15716952790512	3.92736783361255
C	3.27947837237690	-0.79390347059371	3.56761177011368
H	3.62982578331405	-0.63164154533395	4.59970763906628
C	4.11898921013304	-1.41234920199629	2.62784079066959
H	5.13171892677627	-1.73934103878058	2.91157747306886
C	3.66436286964079	-1.59637374453534	1.31054301686272
H	4.34165475108278	-2.05940992916360	0.57634545800460
C	2.37563659060195	-1.16413302491990	0.92612465856932
C	-1.09907228331838	-1.19439825941236	1.61370725020350
C	-1.14313278560968	-1.85216542107016	2.86870141659222
H	-0.41462663345296	-1.57504679106348	3.64764730689651
C	-2.04988326940964	-2.88949738439433	3.14410227245563
H	-2.03646551130150	-3.38336405498261	4.12906339772209
C	-2.95024126934846	-3.31547961231320	2.15452129163772
H	-3.64698820494504	-4.14570947567424	2.35027903929150
C	-2.94545476520422	-2.67613519079423	0.90389698173085
H	-3.64252205008568	-3.02076817974500	0.12408254163290
C	-2.04082208046959	-1.62492870957443	0.63592638331949
C	-0.68962764156041	3.60968770713932	-1.80950453689664
H	-0.47245030110174	4.59993501717952	-1.35579143711045
C	-2.20919499380900	3.44729686764676	-1.89411707374149
H	-2.64453265421097	4.28046853790942	-2.48633250746149
H	-2.69297841839005	3.45055704665609	-0.89853139309570
H	-2.47619700591191	2.50184890418104	-2.40628601236662
C	-0.05898293117316	3.56572978222638	-3.21248732630737
H	-0.23615380997258	2.58140569240647	-3.69352582315855
H	1.03463449244319	3.74493459149735	-3.20383050566711
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C	3.24801430236956	-1.16738905717386	-1.94499071833338
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